



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Feb 12, 2020 – 02:26 PM EST

PDB ID : 6TCL
EMDB ID: : EMD-10461
Title : Photosystem I tetramer
Authors : Chen, M.; Perez-Boerema, A.; Li, S.; Amunts, A.
Deposited on : 2019-11-06
Resolution : 3.20 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

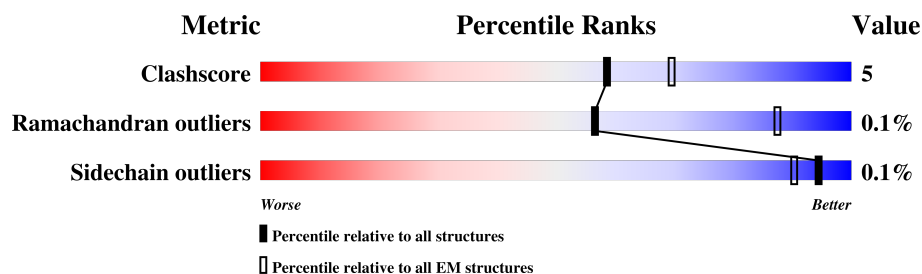
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY










The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






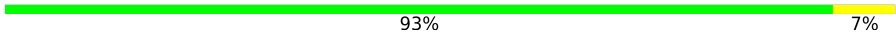
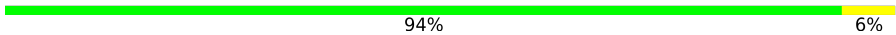

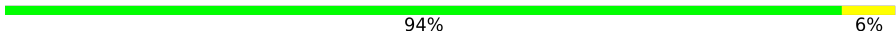






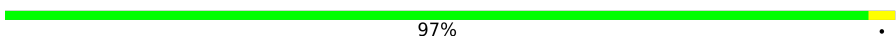
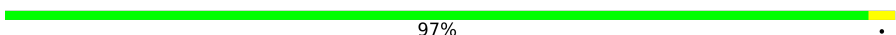





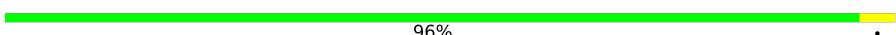



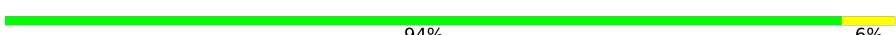
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain	
1	A	740		90% 10%
1	A1	740		89% 11%
1	A2	740		87% 13%
1	AA	740		91% 9%
2	B	739		87% 13%
2	B1	739		86% 14%
2	B2	739		86% 14%
2	BB	739		85% 15%
3	C	80		86% 14%

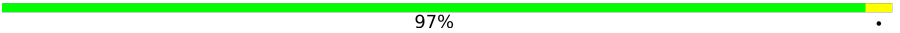
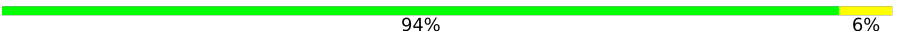



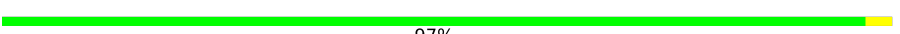








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Mol	Chain	Length	Quality of chain
3	C1	80	 84% 15%
3	C2	80	 88% 11%
3	CC	80	 84% 16%
4	D	134	 93% 7%
4	D1	134	 94% 6%
4	D2	134	 91% 9%
4	DD	134	 94% 6%
5	E1	60	 92% 8%
5	E2	60	 92% 8%
6	F	139	 92% 8%
6	F1	139	 90% 10%
6	FF	139	 88% 12%
7	I	31	 94% 6%
7	I1	31	 97%
7	II	31	 97%
8	J	48	 83% 6% 10%
8	J1	48	 81% 8% 10%
8	J2	48	 79% 10% 10%
8	JJ	48	 77% 13% 10%
9	K	74	 68% 14% 19%
9	K1	74	 96%
9	KK	74	 72% 9% 19%
10	L1	166	 89% 11%
11	M	31	 84% 16%
11	M1	31	 94% 6%

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Mol	Chain	Length	Quality of chain
11	M2	31	 97% .
11	MM	31	 94% 6%
12	X	39	 95% 5%
12	X1	39	 92% 8%
12	X2	39	 90% 10%
12	XX	39	 97% .
13	F2	137	 85% 13% ..
14	I2	33	 94% 6%
15	K2	73	 88% 12%
16	L2	167	 89% 10% .
17	E	63	 90% 10%
17	EE	63	 87% 13%
18	L	154	 95% 5%
18	LL	154	 94% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	801	X	-	-	-
19	CLA	A	804	X	-	-	-
19	CLA	A	805	X	-	-	-
19	CLA	A	806	X	-	-	-
19	CLA	A	807	X	-	-	-
19	CLA	A	808	X	-	-	-
19	CLA	A	809	X	-	-	-
19	CLA	A	810	X	-	-	-
19	CLA	A	811	X	-	-	-
19	CLA	A	812	X	-	-	-
19	CLA	A	813	X	-	-	-
19	CLA	A	814	X	-	-	-
19	CLA	A	815	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	816	X	-	-	-
19	CLA	A	817	X	-	-	-
19	CLA	A	818	X	-	-	-
19	CLA	A	819	X	-	-	-
19	CLA	A	820	X	-	-	-
19	CLA	A	821	X	-	-	-
19	CLA	A	822	X	-	-	-
19	CLA	A	823	X	-	-	-
19	CLA	A	824	X	-	-	-
19	CLA	A	825	X	-	-	-
19	CLA	A	826	X	-	-	-
19	CLA	A	827	X	-	-	-
19	CLA	A	828	X	-	-	-
19	CLA	A	829	X	-	-	-
19	CLA	A	830	X	-	-	-
19	CLA	A	831	X	-	-	-
19	CLA	A	832	X	-	-	-
19	CLA	A	833	X	-	-	-
19	CLA	A	834	X	-	-	-
19	CLA	A	835	X	-	-	-
19	CLA	A	836	X	-	-	-
19	CLA	A	837	X	-	-	-
19	CLA	A	838	X	-	-	-
19	CLA	A	839	X	-	-	-
19	CLA	A	840	X	-	-	-
19	CLA	A	841	X	-	-	-
19	CLA	A	842	X	-	-	-
19	CLA	A	844	X	-	-	-
19	CLA	A	852	X	-	-	-
19	CLA	A1	801	X	-	-	-
19	CLA	A1	803	X	-	-	-
19	CLA	A1	804	X	-	-	-
19	CLA	A1	805	X	-	-	-
19	CLA	A1	806	X	-	-	-
19	CLA	A1	807	X	-	-	-
19	CLA	A1	808	X	-	-	-
19	CLA	A1	809	X	-	-	-
19	CLA	A1	810	X	-	-	-
19	CLA	A1	811	X	-	-	-
19	CLA	A1	812	X	-	-	-
19	CLA	A1	813	X	-	-	-
19	CLA	A1	814	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A1	815	X	-	-	-
19	CLA	A1	816	X	-	-	-
19	CLA	A1	817	X	-	-	-
19	CLA	A1	818	X	-	-	-
19	CLA	A1	819	X	-	-	-
19	CLA	A1	820	X	-	-	-
19	CLA	A1	821	X	-	-	-
19	CLA	A1	822	X	-	-	-
19	CLA	A1	823	X	-	-	-
19	CLA	A1	824	X	-	-	-
19	CLA	A1	825	X	-	-	-
19	CLA	A1	826	X	-	-	-
19	CLA	A1	827	X	-	-	-
19	CLA	A1	828	X	-	-	-
19	CLA	A1	829	X	-	-	-
19	CLA	A1	830	X	-	-	-
19	CLA	A1	831	X	-	-	-
19	CLA	A1	832	X	-	-	-
19	CLA	A1	833	X	-	-	-
19	CLA	A1	834	X	-	-	-
19	CLA	A1	835	X	-	-	-
19	CLA	A1	836	X	-	-	-
19	CLA	A1	837	X	-	-	-
19	CLA	A1	838	X	-	-	-
19	CLA	A1	839	X	-	-	-
19	CLA	A1	840	X	-	-	-
19	CLA	A1	841	X	-	-	-
19	CLA	A1	842	X	-	-	-
19	CLA	A1	844	X	-	-	-
19	CLA	A1	852	X	-	-	-
19	CLA	A2	801	X	-	-	-
19	CLA	A2	802	X	-	-	-
19	CLA	A2	804	X	-	-	-
19	CLA	A2	805	X	-	-	-
19	CLA	A2	806	X	-	-	-
19	CLA	A2	807	X	-	-	-
19	CLA	A2	808	X	-	-	-
19	CLA	A2	809	X	-	-	-
19	CLA	A2	810	X	-	-	-
19	CLA	A2	811	X	-	-	-
19	CLA	A2	812	X	-	-	-
19	CLA	A2	813	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A2	814	X	-	-	-
19	CLA	A2	815	X	-	-	-
19	CLA	A2	816	X	-	-	-
19	CLA	A2	817	X	-	-	-
19	CLA	A2	818	X	-	-	-
19	CLA	A2	819	X	-	-	-
19	CLA	A2	820	X	-	-	-
19	CLA	A2	821	X	-	-	-
19	CLA	A2	822	X	-	-	-
19	CLA	A2	823	X	-	-	-
19	CLA	A2	824	X	-	-	-
19	CLA	A2	825	X	-	-	-
19	CLA	A2	826	X	-	-	-
19	CLA	A2	827	X	-	-	-
19	CLA	A2	828	X	-	-	-
19	CLA	A2	829	X	-	-	-
19	CLA	A2	830	X	-	-	-
19	CLA	A2	831	X	-	-	-
19	CLA	A2	832	X	-	-	-
19	CLA	A2	833	X	-	-	-
19	CLA	A2	834	X	-	-	-
19	CLA	A2	835	X	-	-	-
19	CLA	A2	836	X	-	-	-
19	CLA	A2	837	X	-	-	-
19	CLA	A2	838	X	-	-	-
19	CLA	A2	839	X	-	-	-
19	CLA	A2	840	X	-	-	-
19	CLA	A2	841	X	-	-	-
19	CLA	A2	842	X	-	-	-
19	CLA	A2	844	X	-	-	-
19	CLA	A2	852	X	-	-	-
19	CLA	AA	801	X	-	-	-
19	CLA	AA	804	X	-	-	-
19	CLA	AA	805	X	-	-	-
19	CLA	AA	806	X	-	-	-
19	CLA	AA	807	X	-	-	-
19	CLA	AA	808	X	-	-	-
19	CLA	AA	809	X	-	-	-
19	CLA	AA	810	X	-	-	-
19	CLA	AA	811	X	-	-	-
19	CLA	AA	812	X	-	-	-
19	CLA	AA	813	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	AA	814	X	-	-	-
19	CLA	AA	815	X	-	-	-
19	CLA	AA	816	X	-	-	-
19	CLA	AA	817	X	-	-	-
19	CLA	AA	818	X	-	-	-
19	CLA	AA	819	X	-	-	-
19	CLA	AA	820	X	-	-	-
19	CLA	AA	821	X	-	-	-
19	CLA	AA	822	X	-	-	-
19	CLA	AA	823	X	-	-	-
19	CLA	AA	824	X	-	-	-
19	CLA	AA	825	X	-	-	-
19	CLA	AA	826	X	-	-	-
19	CLA	AA	827	X	-	-	-
19	CLA	AA	828	X	-	-	-
19	CLA	AA	829	X	-	-	-
19	CLA	AA	830	X	-	-	-
19	CLA	AA	831	X	-	-	-
19	CLA	AA	832	X	-	-	-
19	CLA	AA	833	X	-	-	-
19	CLA	AA	834	X	-	-	-
19	CLA	AA	835	X	-	-	-
19	CLA	AA	836	X	-	-	-
19	CLA	AA	837	X	-	-	-
19	CLA	AA	838	X	-	-	-
19	CLA	AA	839	X	-	-	-
19	CLA	AA	840	X	-	-	-
19	CLA	AA	841	X	-	-	-
19	CLA	AA	842	X	-	-	-
19	CLA	AA	843	X	-	-	-
19	CLA	AA	845	X	-	-	-
19	CLA	AA	853	X	-	-	-
19	CLA	B	801	X	-	-	-
19	CLA	B	802	X	-	-	-
19	CLA	B	803	X	-	-	-
19	CLA	B	804	X	-	-	-
19	CLA	B	805	X	-	-	-
19	CLA	B	806	X	-	-	-
19	CLA	B	807	X	-	-	-
19	CLA	B	808	X	-	-	-
19	CLA	B	809	X	-	-	-
19	CLA	B	810	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	811	X	-	-	-
19	CLA	B	812	X	-	-	-
19	CLA	B	813	X	-	-	-
19	CLA	B	814	X	-	-	-
19	CLA	B	815	X	-	-	-
19	CLA	B	816	X	-	-	-
19	CLA	B	817	X	-	-	-
19	CLA	B	818	X	-	-	-
19	CLA	B	819	X	-	-	-
19	CLA	B	820	X	-	-	-
19	CLA	B	821	X	-	-	-
19	CLA	B	822	X	-	-	-
19	CLA	B	823	X	-	-	-
19	CLA	B	824	X	-	-	-
19	CLA	B	825	X	-	-	-
19	CLA	B	826	X	-	-	-
19	CLA	B	827	X	-	-	-
19	CLA	B	828	X	-	-	-
19	CLA	B	829	X	-	-	-
19	CLA	B	830	X	-	-	-
19	CLA	B	831	X	-	-	-
19	CLA	B	832	X	-	-	-
19	CLA	B	833	X	-	-	-
19	CLA	B	834	X	-	-	-
19	CLA	B	835	X	-	-	-
19	CLA	B	836	X	-	-	-
19	CLA	B	837	X	-	-	-
19	CLA	B	846	X	-	-	-
19	CLA	B	854	X	-	-	-
19	CLA	B	858	X	-	-	-
19	CLA	B	859	X	-	-	-
19	CLA	B	860	X	-	-	-
19	CLA	B1	801	X	-	-	-
19	CLA	B1	802	X	-	-	-
19	CLA	B1	803	X	-	-	-
19	CLA	B1	804	X	-	-	-
19	CLA	B1	805	X	-	-	-
19	CLA	B1	806	X	-	-	-
19	CLA	B1	807	X	-	-	-
19	CLA	B1	808	X	-	-	-
19	CLA	B1	809	X	-	-	-
19	CLA	B1	810	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B1	811	X	-	-	-
19	CLA	B1	812	X	-	-	-
19	CLA	B1	813	X	-	-	-
19	CLA	B1	814	X	-	-	-
19	CLA	B1	815	X	-	-	-
19	CLA	B1	816	X	-	-	-
19	CLA	B1	817	X	-	-	-
19	CLA	B1	818	X	-	-	-
19	CLA	B1	819	X	-	-	-
19	CLA	B1	820	X	-	-	-
19	CLA	B1	821	X	-	-	-
19	CLA	B1	822	X	-	-	-
19	CLA	B1	823	X	-	-	-
19	CLA	B1	824	X	-	-	-
19	CLA	B1	825	X	-	-	-
19	CLA	B1	826	X	-	-	-
19	CLA	B1	827	X	-	-	-
19	CLA	B1	828	X	-	-	-
19	CLA	B1	829	X	-	-	-
19	CLA	B1	830	X	-	-	-
19	CLA	B1	831	X	-	-	-
19	CLA	B1	832	X	-	-	-
19	CLA	B1	833	X	-	-	-
19	CLA	B1	834	X	-	-	-
19	CLA	B1	835	X	-	-	-
19	CLA	B1	836	X	-	-	-
19	CLA	B1	845	X	-	-	-
19	CLA	B1	848	X	-	-	-
19	CLA	B1	849	X	-	-	-
19	CLA	B1	850	X	-	-	-
19	CLA	B2	801	X	-	-	-
19	CLA	B2	802	X	-	-	-
19	CLA	B2	803	X	-	-	-
19	CLA	B2	804	X	-	-	-
19	CLA	B2	805	X	-	-	-
19	CLA	B2	806	X	-	-	-
19	CLA	B2	807	X	-	-	-
19	CLA	B2	808	X	-	-	-
19	CLA	B2	809	X	-	-	-
19	CLA	B2	810	X	-	-	-
19	CLA	B2	811	X	-	-	-
19	CLA	B2	812	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B2	813	X	-	-	-
19	CLA	B2	814	X	-	-	-
19	CLA	B2	815	X	-	-	-
19	CLA	B2	816	X	-	-	-
19	CLA	B2	817	X	-	-	-
19	CLA	B2	818	X	-	-	-
19	CLA	B2	819	X	-	-	-
19	CLA	B2	820	X	-	-	-
19	CLA	B2	821	X	-	-	-
19	CLA	B2	822	X	-	-	-
19	CLA	B2	823	X	-	-	-
19	CLA	B2	824	X	-	-	-
19	CLA	B2	825	X	-	-	-
19	CLA	B2	826	X	-	-	-
19	CLA	B2	827	X	-	-	-
19	CLA	B2	828	X	-	-	-
19	CLA	B2	829	X	-	-	-
19	CLA	B2	830	X	-	-	-
19	CLA	B2	831	X	-	-	-
19	CLA	B2	832	X	-	-	-
19	CLA	B2	833	X	-	-	-
19	CLA	B2	834	X	-	-	-
19	CLA	B2	835	X	-	-	-
19	CLA	B2	836	X	-	-	-
19	CLA	B2	837	X	-	-	-
19	CLA	B2	846	X	-	-	-
19	CLA	B2	849	X	-	-	-
19	CLA	B2	850	X	-	-	-
19	CLA	B2	851	X	-	-	-
19	CLA	B2	852	X	-	-	-
19	CLA	BB	801	X	-	-	-
19	CLA	BB	802	X	-	-	-
19	CLA	BB	803	X	-	-	-
19	CLA	BB	804	X	-	-	-
19	CLA	BB	805	X	-	-	-
19	CLA	BB	806	X	-	-	-
19	CLA	BB	807	X	-	-	-
19	CLA	BB	808	X	-	-	-
19	CLA	BB	809	X	-	-	-
19	CLA	BB	810	X	-	-	-
19	CLA	BB	811	X	-	-	-
19	CLA	BB	812	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	BB	813	X	-	-	-
19	CLA	BB	814	X	-	-	-
19	CLA	BB	815	X	-	-	-
19	CLA	BB	816	X	-	-	-
19	CLA	BB	817	X	-	-	-
19	CLA	BB	818	X	-	-	-
19	CLA	BB	819	X	-	-	-
19	CLA	BB	820	X	-	-	-
19	CLA	BB	821	X	-	-	-
19	CLA	BB	822	X	-	-	-
19	CLA	BB	823	X	-	-	-
19	CLA	BB	824	X	-	-	-
19	CLA	BB	825	X	-	-	-
19	CLA	BB	826	X	-	-	-
19	CLA	BB	827	X	-	-	-
19	CLA	BB	828	X	-	-	-
19	CLA	BB	829	X	-	-	-
19	CLA	BB	830	X	-	-	-
19	CLA	BB	831	X	-	-	-
19	CLA	BB	832	X	-	-	-
19	CLA	BB	833	X	-	-	-
19	CLA	BB	834	X	-	-	-
19	CLA	BB	835	X	-	-	-
19	CLA	BB	836	X	-	-	-
19	CLA	BB	845	X	-	-	-
19	CLA	BB	852	X	-	-	-
19	CLA	BB	855	X	-	-	-
19	CLA	BB	856	X	-	-	-
19	CLA	F	301	X	-	-	-
19	CLA	F	302	X	-	-	-
19	CLA	F1	301	X	-	-	-
19	CLA	F1	302	X	-	-	-
19	CLA	F1	305	X	-	-	-
19	CLA	F2	301	X	-	-	-
19	CLA	F2	302	X	-	-	-
19	CLA	FF	301	X	-	-	-
19	CLA	FF	302	X	-	-	-
19	CLA	FF	305	X	-	-	-
19	CLA	J	101	X	-	-	-
19	CLA	J	103	X	-	-	-
19	CLA	J1	101	X	-	-	-
19	CLA	J1	103	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	J2	101	X	-	-	-
19	CLA	J2	103	X	-	-	-
19	CLA	JJ	101	X	-	-	-
19	CLA	JJ	103	X	-	-	-
19	CLA	K	101	X	-	-	-
19	CLA	K	102	X	-	-	-
19	CLA	K1	102	X	-	-	-
19	CLA	K1	103	X	-	-	-
19	CLA	K1	105	X	-	-	-
19	CLA	K2	102	X	-	-	-
19	CLA	K2	104	X	-	-	-
19	CLA	KK	101	X	-	-	-
19	CLA	KK	102	X	-	-	-
19	CLA	L	202	X	-	-	-
19	CLA	L	203	X	-	-	-
19	CLA	L	204	X	-	-	-
19	CLA	L1	205	X	-	-	-
19	CLA	L1	206	X	-	-	-
19	CLA	L1	207	X	-	-	-
19	CLA	L2	204	X	-	-	-
19	CLA	L2	205	X	-	-	-
19	CLA	L2	206	X	-	-	-
19	CLA	LL	201	X	-	-	-
19	CLA	LL	202	X	-	-	-
19	CLA	LL	203	X	-	-	-
19	CLA	X	101	X	-	-	-
19	CLA	X1	101	X	-	-	-
19	CLA	X2	101	X	-	-	-
19	CLA	XX	101	X	-	-	-
20	CL0	A	803	X	-	-	-
20	CL0	A1	802	X	-	-	-
20	CL0	A2	803	X	-	-	-
20	CL0	AA	803	X	-	-	-
24	AJP	A	802	X	-	-	-
24	AJP	AA	802	X	-	-	-
24	AJP	B	849	X	-	-	-
24	AJP	B	850	X	-	-	-
24	AJP	BB	848	X	-	-	-
24	AJP	BB	849	X	-	-	-
24	AJP	I2	104	X	-	-	-
24	AJP	K	104	X	-	-	-
24	AJP	KK	104	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	AJP	L	208	X	-	-	-
24	AJP	L	209	X	-	-	-
24	AJP	L1	203	X	-	-	-
24	AJP	L1	204	X	-	-	-
24	AJP	L2	202	X	-	-	-
24	AJP	L2	203	X	-	-	-
24	AJP	M2	101	X	-	-	-

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 199181 atoms, of which 99577 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A1	740	Total	C	H	N	O	S	0	0
			11478	3809	5672	1000	976	21		
1	A2	740	Total	C	H	N	O	S	0	0
			11486	3809	5680	1000	976	21		
1	A	740	Total	C	H	N	O	S	0	0
			11483	3809	5677	1000	976	21		
1	AA	740	Total	C	H	N	O	S	0	0
			11483	3809	5677	1000	976	21		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B1	739	Total	C	H	N	O	S	0	0
			11579	3905	5660	990	1006	18		
2	B2	739	Total	C	H	N	O	S	0	0
			11581	3905	5662	990	1006	18		
2	B	739	Total	C	H	N	O	S	0	0
			11586	3905	5667	990	1006	18		
2	BB	739	Total	C	H	N	O	S	0	0
			11595	3905	5676	990	1006	18		

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C1	80	Total	C	H	N	O	S	0	0
			1183	367	584	103	118	11		
3	C2	80	Total	C	H	N	O	S	0	0
			1179	367	580	103	118	11		
3	C	80	Total	C	H	N	O	S	0	0
			1181	367	582	103	118	11		
3	CC	80	Total	C	H	N	O	S	0	0
			1181	367	582	103	118	11		

- Molecule 4 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D1	134	Total	C	H	N	O	S	0	0
			2073	664	1037	178	193	1		
4	D2	134	Total	C	H	N	O	S	0	0
			2078	664	1042	178	193	1		
4	D	134	Total	C	H	N	O	S	0	0
			2078	664	1042	178	193	1		
4	DD	134	Total	C	H	N	O	S	0	0
			2078	664	1042	178	193	1		

- Molecule 5 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E1	60	Total	C	H	N	O		0	0
			958	308	477	83	90			
5	E2	60	Total	C	H	N	O		0	0
			958	308	477	83	90			

- Molecule 6 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F1	139	Total	C	H	N	O	S	0	0
			2112	678	1052	179	201	2		
6	F	139	Total	C	H	N	O	S	0	0
			2111	678	1051	179	201	2		
6	FF	139	Total	C	H	N	O	S	0	0
			2112	678	1052	179	201	2		

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	I1	31	Total	C	H	N	O		0	0
			508	177	255	35	41			
7	I	31	Total	C	H	N	O		0	0
			508	177	255	35	41			
7	II	31	Total	C	H	N	O		0	0
			508	177	255	35	41			

- Molecule 8 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	J1	43	Total	C	H	N	O		0	0
			701	237	355	52	57			

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	J2	43	Total	C	H	N	O	0	0
			701	237	355	52	57		
8	J	43	Total	C	H	N	O	0	0
			701	237	355	52	57		
8	JJ	43	Total	C	H	N	O	0	0
			700	237	354	52	57		

- Molecule 9 is a protein called Photosystem I reaction center subunit Psal 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	K1	74	Total	C	H	N	O	S	0	0
			1091	356	555	87	92	1		
9	K	60	Total	C	H	N	O	S	0	0
			900	289	461	72	77	1		
9	KK	60	Total	C	H	N	O	S	0	0
			900	289	461	72	77	1		

- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace	
10	L1	166	Total	C	H	N	O	S	0	0
			2483	810	1239	213	220	1		

- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M1	31	Total	C	H	N	O	0	0
			496	160	256	37	43		
11	M2	31	Total	C	H	N	O	0	0
			496	160	256	37	43		
11	M	31	Total	C	H	N	O	0	0
			496	160	256	37	43		
11	MM	31	Total	C	H	N	O	0	0
			496	160	256	37	43		

- Molecule 12 is a protein called Photosystem I 4.8 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	X1	39	Total	C	H	N	O	0	0
			627	212	318	49	48		
12	X2	39	Total	C	H	N	O	0	0
			627	212	318	49	48		

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Mol	Chain	Residues	Atoms					AltConf	Trace
12	X	39	Total	C	H	N	O	0	0
			628	212	319	49	48		
12	XX	39	Total	C	H	N	O	0	0
			628	212	319	49	48		

- Molecule 13 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	F2	137	Total	C	H	N	O	S	0	0
			2087	670	1040	177	198	2		

- Molecule 14 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I2	33	Total	C	H	N	O	0	0
			536	186	268	37	45		

- Molecule 15 is a protein called Photosystem I reaction center subunit Psak 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	K2	73	Total	C	H	N	O	S	0	0
			1081	353	550	86	91	1		

- Molecule 16 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	L2	167	Total	C	H	N	O	S	0	0
			2498	815	1245	215	222	1		

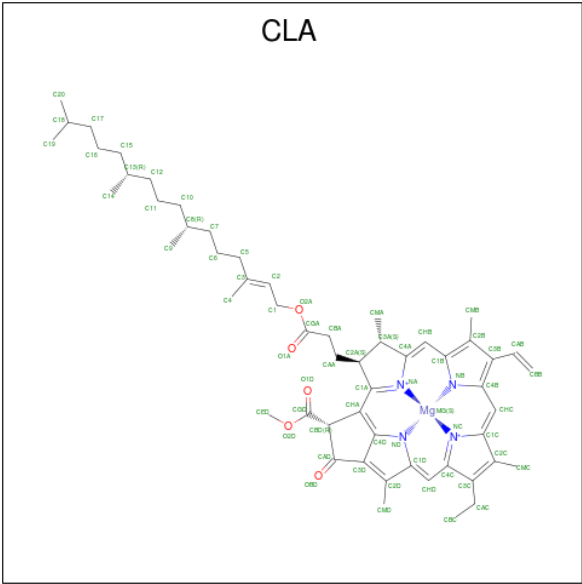
- Molecule 17 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	E	63	Total	C	H	N	O	0	0
			994	321	492	86	95		
17	EE	63	Total	C	H	N	O	0	0
			994	321	492	86	95		

- Molecule 18 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	L	154	Total	C	H	N	O	S	0	0
			2309	758	1153	196	201	1		
18	LL	154	Total	C	H	N	O	S	0	0
			2310	758	1154	196	201	1		

- Molecule 19 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms						AltConf
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	

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Mol	Chain	Residues	Atoms						AltConf
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	

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Mol	Chain	Residues	Atoms						AltConf
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	F1	1	Total	C	H	Mg	N	O	0
			269	119	122	3	12	13	
19	F1	1	Total	C	H	Mg	N	O	0
			269	119	122	3	12	13	
19	F1	1	Total	C	H	Mg	N	O	0
			269	119	122	3	12	13	
19	J1	1	Total	C	H	Mg	N	O	0
			139	66	57	2	8	6	
19	J1	1	Total	C	H	Mg	N	O	0
			139	66	57	2	8	6	
19	K1	1	Total	C	H	Mg	N	O	0
			223	103	92	3	12	13	
19	K1	1	Total	C	H	Mg	N	O	0
			223	103	92	3	12	13	
19	K1	1	Total	C	H	Mg	N	O	0
			223	103	92	3	12	13	
19	L1	1	Total	C	H	Mg	N	O	0
			393	161	202	3	12	15	
19	L1	1	Total	C	H	Mg	N	O	0
			393	161	202	3	12	15	
19	L1	1	Total	C	H	Mg	N	O	0
			393	161	202	3	12	15	

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Mol	Chain	Residues	Atoms						AltConf
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	F2	1	Total	C	H	Mg	N	O	0
			191	84	89	2	8	8	
19	F2	1	Total	C	H	Mg	N	O	0
			191	84	89	2	8	8	
19	J2	1	Total	C	H	Mg	N	O	0
			140	66	58	2	8	6	
19	J2	1	Total	C	H	Mg	N	O	0
			140	66	58	2	8	6	
19	K2	1	Total	C	H	Mg	N	O	0
			147	68	61	2	8	8	
19	K2	1	Total	C	H	Mg	N	O	0
			147	68	61	2	8	8	
19	L2	1	Total	C	H	Mg	N	O	0
			373	156	187	3	12	15	
19	L2	1	Total	C	H	Mg	N	O	0
			373	156	187	3	12	15	
19	L2	1	Total	C	H	Mg	N	O	0
			373	156	187	3	12	15	
19	X2	1	Total	C	H	Mg	N	O	0
			77	35	32	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	

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Mol	Chain	Residues	Atoms						AltConf
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0

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Mol	Chain	Residues	Atoms						AltConf
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	B	1	Total 4758	C 1995	H 2357	Mg 42	N 168	O 196	0
19	B	1	Total 4758	C 1995	H 2357	Mg 42	N 168	O 196	0
19	B	1	Total 4758	C 1995	H 2357	Mg 42	N 168	O 196	0
19	B	1	Total 4758	C 1995	H 2357	Mg 42	N 168	O 196	0
19	B	1	Total 4758	C 1995	H 2357	Mg 42	N 168	O 196	0
19	B	1	Total 4758	C 1995	H 2357	Mg 42	N 168	O 196	0
19	B	1	Total 4758	C 1995	H 2357	Mg 42	N 168	O 196	0
19	B	1	Total 4758	C 1995	H 2357	Mg 42	N 168	O 196	0
19	B	1	Total 4758	C 1995	H 2357	Mg 42	N 168	O 196	0

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Mol	Chain	Residues	Atoms						AltConf
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	F	1	Total	C	H	Mg	N	O	0
			191	84	89	2	8	8	
19	F	1	Total	C	H	Mg	N	O	0
			191	84	89	2	8	8	
19	J	1	Total	C	H	Mg	N	O	0
			140	66	58	2	8	6	
19	J	1	Total	C	H	Mg	N	O	0
			140	66	58	2	8	6	
19	K	1	Total	C	H	Mg	N	O	0
			156	71	65	2	8	10	
19	K	1	Total	C	H	Mg	N	O	0
			156	71	65	2	8	10	
19	L	1	Total	C	H	Mg	N	O	0
			389	161	198	3	12	15	
19	L	1	Total	C	H	Mg	N	O	0
			389	161	198	3	12	15	
19	L	1	Total	C	H	Mg	N	O	0
			389	161	198	3	12	15	

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Mol	Chain	Residues	Atoms						AltConf
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0

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Mol	Chain	Residues	Atoms						AltConf
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0

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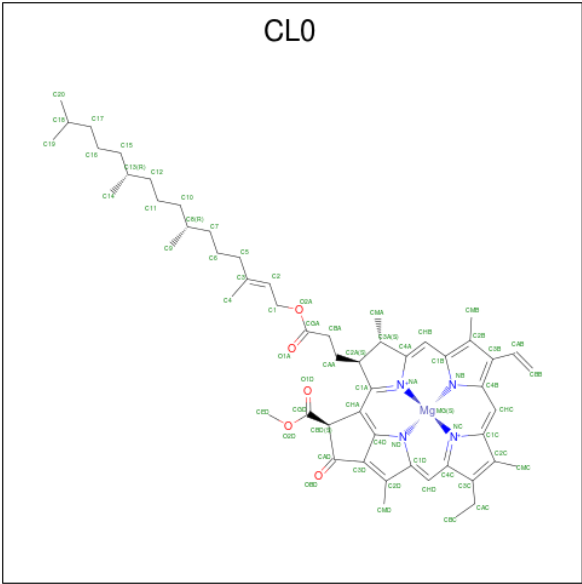
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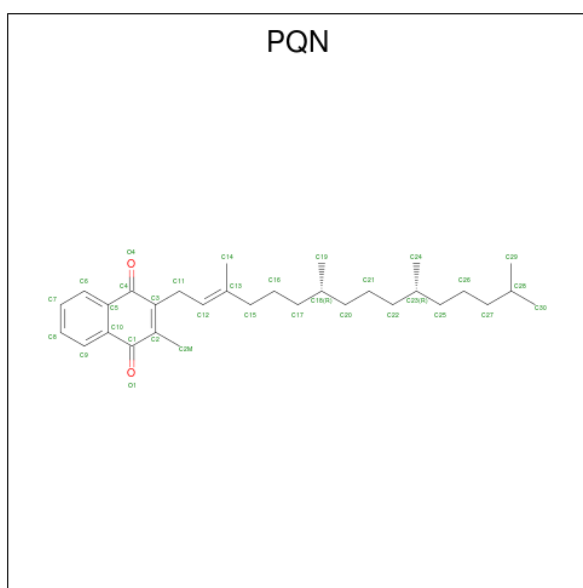
Mol	Chain	Residues	Atoms						AltConf
19	FF	1	Total	C	H	Mg	N	O	0
			328	139	161	3	12	13	
19	FF	1	Total	C	H	Mg	N	O	0
			328	139	161	3	12	13	
19	FF	1	Total	C	H	Mg	N	O	0
			328	139	161	3	12	13	
19	JJ	1	Total	C	H	Mg	N	O	0
			139	66	57	2	8	6	
19	JJ	1	Total	C	H	Mg	N	O	0
			139	66	57	2	8	6	
19	KK	1	Total	C	H	Mg	N	O	0
			156	71	65	2	8	10	
19	KK	1	Total	C	H	Mg	N	O	0
			156	71	65	2	8	10	
19	LL	1	Total	C	H	Mg	N	O	0
			323	140	155	3	12	13	
19	LL	1	Total	C	H	Mg	N	O	0
			323	140	155	3	12	13	
19	LL	1	Total	C	H	Mg	N	O	0
			323	140	155	3	12	13	
19	XX	1	Total	C	H	Mg	N	O	0
			77	35	32	1	4	5	

- Molecule 20 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅).



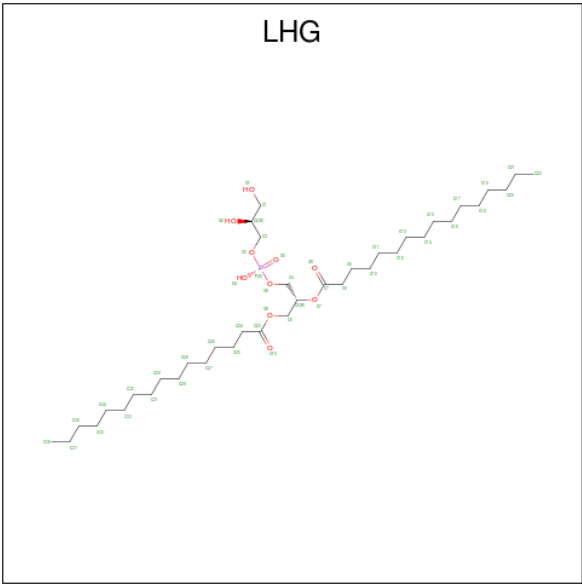
Mol	Chain	Residues	Atoms						AltConf
20	A1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
20	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
20	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
20	AA	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

- Molecule 21 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms				AltConf
21	A1	1	Total	C	H	O	0
			79	31	46	2	
21	B1	1	Total	C	H	O	0
			79	31	46	2	
21	A2	1	Total	C	H	O	0
			79	31	46	2	
21	B2	1	Total	C	H	O	0
			79	31	46	2	
21	A	1	Total	C	H	O	0
			79	31	46	2	
21	B	1	Total	C	H	O	0
			79	31	46	2	
21	AA	1	Total	C	H	O	0
			79	31	46	2	
21	BB	1	Total	C	H	O	0
			79	31	46	2	

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by author).



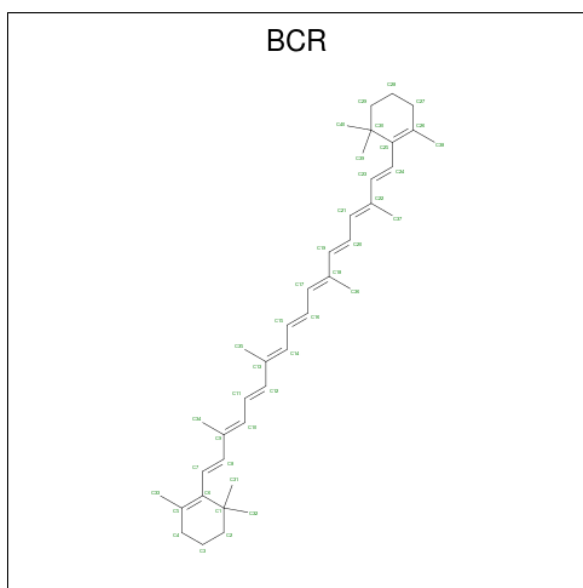
Mol	Chain	Residues	Atoms					AltConf
22	A1	1	Total	C	H	O	P	0
			209	65	122	20	2	
22	A1	1	Total	C	H	O	P	0
			209	65	122	20	2	
22	B1	1	Total	C	H	O	P	0
			69	22	36	10	1	
22	L1	1	Total	C	H	O	P	0
			68	22	35	10	1	
22	X1	1	Total	C	H	O	P	0
			212	67	123	20	2	
22	X1	1	Total	C	H	O	P	0
			212	67	123	20	2	
22	A2	1	Total	C	H	O	P	0
			209	65	122	20	2	
22	A2	1	Total	C	H	O	P	0
			209	65	122	20	2	
22	B2	1	Total	C	H	O	P	0
			69	22	36	10	1	
22	L2	1	Total	C	H	O	P	0
			74	24	39	10	1	
22	X2	1	Total	C	H	O	P	0
			212	67	123	20	2	
22	X2	1	Total	C	H	O	P	0
			212	67	123	20	2	

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	H	O	P	0
			209	65	122	20	2	
22	A	1	Total	C	H	O	P	0
			209	65	122	20	2	
22	B	1	Total	C	H	O	P	0
			192	60	110	20	2	
22	B	1	Total	C	H	O	P	0
			192	60	110	20	2	
22	L	1	Total	C	H	O	P	0
			76	23	42	10	1	
22	X	1	Total	C	H	O	P	0
			89	29	49	10	1	
22	AA	1	Total	C	H	O	P	0
			209	65	122	20	2	
22	AA	1	Total	C	H	O	P	0
			209	65	122	20	2	
22	BB	1	Total	C	H	O	P	0
			192	60	110	20	2	
22	BB	1	Total	C	H	O	P	0
			192	60	110	20	2	
22	LL	1	Total	C	H	O	P	0
			76	23	42	10	1	
22	XX	1	Total	C	H	O	P	0
			89	29	49	10	1	

- Molecule 23 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms			AltConf
23	A1	1	Total	C	H	0
			572	239	333	
23	A1	1	Total	C	H	0
			572	239	333	
23	A1	1	Total	C	H	0
			572	239	333	
23	A1	1	Total	C	H	0
			572	239	333	
23	A1	1	Total	C	H	0
			572	239	333	
23	A1	1	Total	C	H	0
			572	239	333	
23	B1	1	Total	C	H	0
			480	200	280	
23	B1	1	Total	C	H	0
			480	200	280	
23	B1	1	Total	C	H	0
			480	200	280	
23	B1	1	Total	C	H	0
			480	200	280	
23	B1	1	Total	C	H	0
			480	200	280	
23	F1	1	Total	C	H	0
			283	120	163	
23	F1	1	Total	C	H	0
			283	120	163	
23	F1	1	Total	C	H	0
			283	120	163	
23	I1	1	Total	C	H	0
			96	40	56	
23	J1	1	Total	C	H	0
			192	80	112	
23	J1	1	Total	C	H	0
			192	80	112	
23	K1	1	Total	C	H	0
			192	80	112	
23	K1	1	Total	C	H	0
			192	80	112	
23	L1	1	Total	C	H	0
			288	120	168	
23	L1	1	Total	C	H	0
			288	120	168	
23	L1	1	Total	C	H	0
			288	120	168	

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Mol	Chain	Residues	Atoms			AltConf
23	M1	1	Total	C	H	0
			96	40	56	
23	A2	1	Total	C	H	0
			572	239	333	
23	A2	1	Total	C	H	0
			572	239	333	
23	A2	1	Total	C	H	0
			572	239	333	
23	A2	1	Total	C	H	0
			572	239	333	
23	A2	1	Total	C	H	0
			572	239	333	
23	A2	1	Total	C	H	0
			572	239	333	
23	B2	1	Total	C	H	0
			475	200	275	
23	B2	1	Total	C	H	0
			475	200	275	
23	B2	1	Total	C	H	0
			475	200	275	
23	B2	1	Total	C	H	0
			475	200	275	
23	B2	1	Total	C	H	0
			475	200	275	
23	F2	1	Total	C	H	0
			283	120	163	
23	F2	1	Total	C	H	0
			283	120	163	
23	F2	1	Total	C	H	0
			283	120	163	
23	I2	1	Total	C	H	0
			288	120	168	
23	I2	1	Total	C	H	0
			288	120	168	
23	I2	1	Total	C	H	0
			288	120	168	
23	J2	1	Total	C	H	0
			192	80	112	
23	J2	1	Total	C	H	0
			192	80	112	
23	K2	1	Total	C	H	0
			192	80	112	

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Mol	Chain	Residues	Atoms			AltConf
23	K2	1	Total	C	H	0
			192	80	112	
23	L2	1	Total	C	H	0
			96	40	56	
23	M2	1	Total	C	H	0
			96	40	56	
23	A	1	Total	C	H	0
			668	279	389	
23	A	1	Total	C	H	0
			668	279	389	
23	A	1	Total	C	H	0
			668	279	389	
23	A	1	Total	C	H	0
			668	279	389	
23	A	1	Total	C	H	0
			668	279	389	
23	A	1	Total	C	H	0
			668	279	389	
23	B	1	Total	C	H	0
			576	240	336	
23	B	1	Total	C	H	0
			576	240	336	
23	B	1	Total	C	H	0
			576	240	336	
23	B	1	Total	C	H	0
			576	240	336	
23	B	1	Total	C	H	0
			576	240	336	
23	B	1	Total	C	H	0
			576	240	336	
23	F	1	Total	C	H	0
			283	120	163	
23	F	1	Total	C	H	0
			283	120	163	
23	F	1	Total	C	H	0
			283	120	163	
23	I	1	Total	C	H	0
			192	80	112	
23	I	1	Total	C	H	0
			192	80	112	

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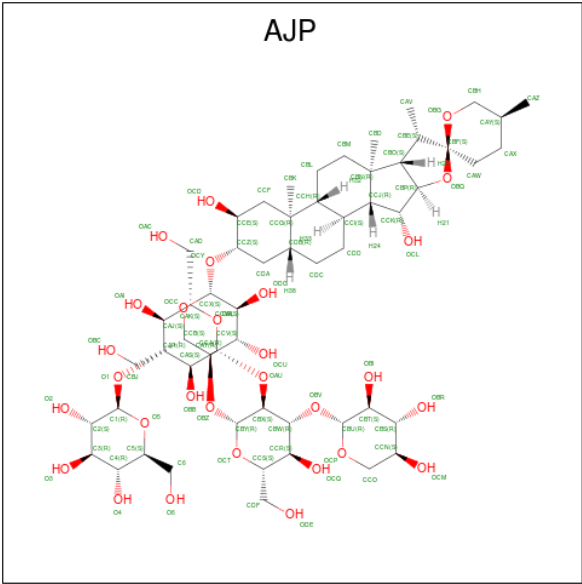
Mol	Chain	Residues	Atoms			AltConf
23	J	1	Total	C	H	0
			192	80	112	
23	J	1	Total	C	H	0
			192	80	112	
23	K	1	Total	C	H	0
			96	40	56	
23	L	1	Total	C	H	0
			192	80	112	
23	L	1	Total	C	H	0
			192	80	112	
23	M	1	Total	C	H	0
			91	40	51	
23	AA	1	Total	C	H	0
			668	279	389	
23	AA	1	Total	C	H	0
			668	279	389	
23	AA	1	Total	C	H	0
			668	279	389	
23	AA	1	Total	C	H	0
			668	279	389	
23	AA	1	Total	C	H	0
			668	279	389	
23	AA	1	Total	C	H	0
			668	279	389	
23	AA	1	Total	C	H	0
			668	279	389	
23	BB	1	Total	C	H	0
			576	240	336	
23	BB	1	Total	C	H	0
			576	240	336	
23	BB	1	Total	C	H	0
			576	240	336	
23	BB	1	Total	C	H	0
			576	240	336	
23	BB	1	Total	C	H	0
			576	240	336	
23	BB	1	Total	C	H	0
			576	240	336	
23	FF	1	Total	C	H	0
			283	120	163	
23	FF	1	Total	C	H	0
			283	120	163	

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	H	
23	FF	1	283	120	163	0
23	II	1	288	120	168	0
23	II	1	288	120	168	0
23	II	1	288	120	168	0
23	JJ	1	192	80	112	0
23	JJ	1	192	80	112	0
23	KK	1	96	40	56	0
23	LL	1	96	40	56	0
23	MM	1	93	40	53	0

- Molecule 24 is Digitonin (three-letter code: AJP) (formula: C₅₆H₉₂O₂₉).



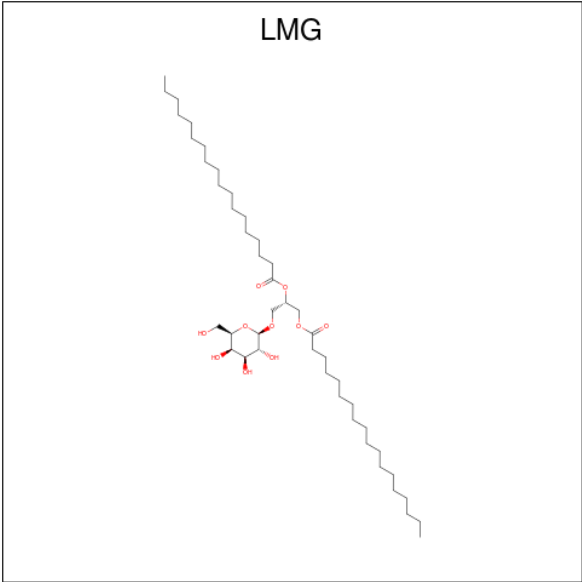
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
24	A1	1	171	60	96	15	0
24	A1	1	171	60	96	15	0

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Mol	Chain	Residues	Atoms				AltConf
24	L1	1	Total	C	H	O	0
			192	66	106	20	
24	L1	1	Total	C	H	O	0
			192	66	106	20	
24	A2	1	Total	C	H	O	0
			75	27	43	5	
24	I2	1	Total	C	H	O	0
			73	27	42	4	
24	L2	1	Total	C	H	O	0
			192	66	106	20	
24	L2	1	Total	C	H	O	0
			192	66	106	20	
24	M2	1	Total	C	H	O	0
			74	27	43	4	
24	A	1	Total	C	H	O	0
			153	56	88	9	
24	A	1	Total	C	H	O	0
			153	56	88	9	
24	B	1	Total	C	H	O	0
			288	99	159	30	
24	B	1	Total	C	H	O	0
			288	99	159	30	
24	B	1	Total	C	H	O	0
			288	99	159	30	
24	K	1	Total	C	H	O	0
			91	32	50	9	
24	L	1	Total	C	H	O	0
			147	54	85	8	
24	L	1	Total	C	H	O	0
			147	54	85	8	
24	AA	1	Total	C	H	O	0
			153	56	88	9	
24	AA	1	Total	C	H	O	0
			153	56	88	9	
24	BB	1	Total	C	H	O	0
			192	66	106	20	
24	BB	1	Total	C	H	O	0
			192	66	106	20	
24	KK	1	Total	C	H	O	0
			91	32	50	9	

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by author).



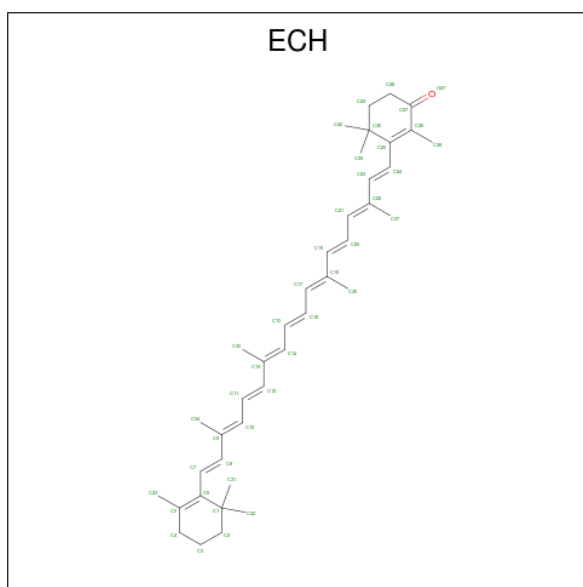
Mol	Chain	Residues	Atoms				AltConf
25	A1	1	Total	C	H	O	1
			152	48	84	20	
25	A1	1	Total	C	H	O	1
			152	48	84	20	
25	B1	1	Total	C	H	O	0
			265	87	148	30	
25	B1	1	Total	C	H	O	0
			265	87	148	30	
25	B1	1	Total	C	H	O	0
			265	87	148	30	
25	I1	1	Total	C	H	O	0
			75	25	40	10	
25	K1	1	Total	C	H	O	1
			120	38	62	20	
25	K1	1	Total	C	H	O	1
			120	38	62	20	
25	L1	1	Total	C	H	O	1
			223	71	132	20	
25	L1	1	Total	C	H	O	0
			223	71	132	20	
25	A2	1	Total	C	H	O	1
			171	54	97	20	
25	A2	1	Total	C	H	O	1
			171	54	97	20	
25	B2	1	Total	C	H	O	0
			265	87	148	30	
25	B2	1	Total	C	H	O	0
			265	87	148	30	

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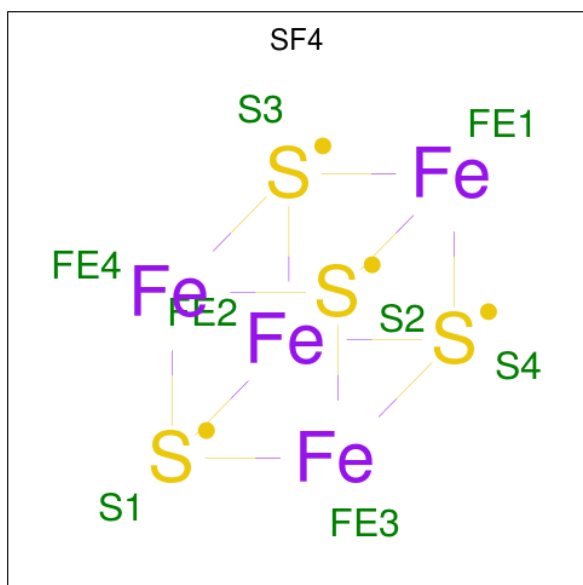
Mol	Chain	Residues	Atoms				AltConf
25	B2	1	Total	C	H	O	0
			265	87	148	30	
25	I2	1	Total	C	H	O	0
			75	25	40	10	
25	K2	1	Total	C	H	O	1
			114	36	58	20	
25	K2	1	Total	C	H	O	1
			114	36	58	20	
25	L2	1	Total	C	H	O	1
			82	26	46	10	
25	B	1	Total	C	H	O	0
			427	136	251	40	
25	B	1	Total	C	H	O	1
			427	136	251	40	
25	B	1	Total	C	H	O	0
			427	136	251	40	
25	B	1	Total	C	H	O	1
			427	136	251	40	
25	L	1	Total	C	H	O	1
			85	27	48	10	
25	M	1	Total	C	H	O	0
			105	36	59	10	
25	BB	1	Total	C	H	O	0
			289	92	167	30	
25	BB	1	Total	C	H	O	1
			289	92	167	30	
25	BB	1	Total	C	H	O	1
			289	92	167	30	
25	II	1	Total	C	H	O	1
			181	59	102	20	
25	II	1	Total	C	H	O	0
			181	59	102	20	

- Molecule 26 is beta,beta-caroten-4-one (three-letter code: ECH) (formula: C₄₀H₅₄O).



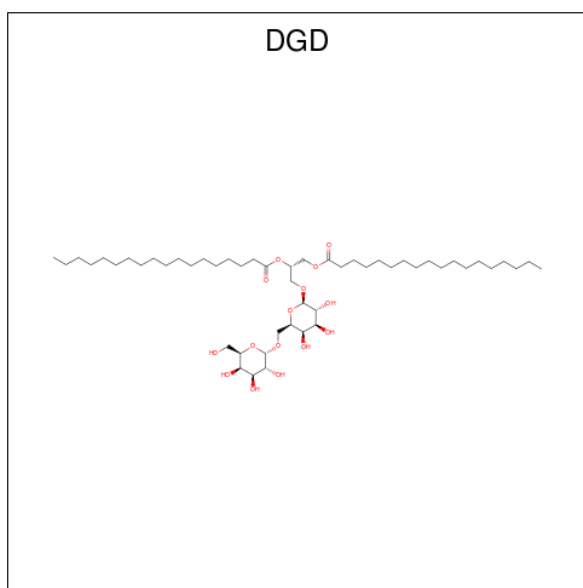
Mol	Chain	Residues	Atoms				AltConf
26	B1	1	Total	C	H	O	0
			95	40	54	1	
26	B2	1	Total	C	H	O	0
			95	40	54	1	
26	B	1	Total	C	H	O	0
			95	40	54	1	
26	BB	1	Total	C	H	O	0
			95	40	54	1	

- Molecule 27 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
27	B1	1	Total	Fe	S	0
			8	4	4	
27	C1	1	Total	Fe	S	0
			16	8	8	
27	C1	1	Total	Fe	S	0
			16	8	8	
27	B2	1	Total	Fe	S	0
			8	4	4	
27	C2	1	Total	Fe	S	0
			16	8	8	
27	C2	1	Total	Fe	S	0
			16	8	8	
27	B	1	Total	Fe	S	0
			8	4	4	
27	C	1	Total	Fe	S	0
			16	8	8	
27	C	1	Total	Fe	S	0
			16	8	8	
27	BB	1	Total	Fe	S	0
			8	4	4	
27	CC	1	Total	Fe	S	0
			16	8	8	
27	CC	1	Total	Fe	S	0
			16	8	8	

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by author).

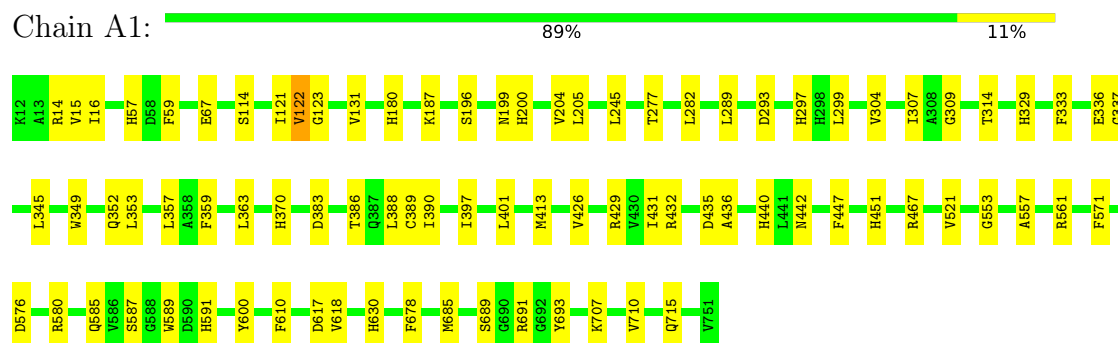


Mol	Chain	Residues	Atoms				AltConf
28	B	1	Total	C	H	O	0
			88	27	46	15	
28	BB	1	Total	C	H	O	0
			88	27	46	15	

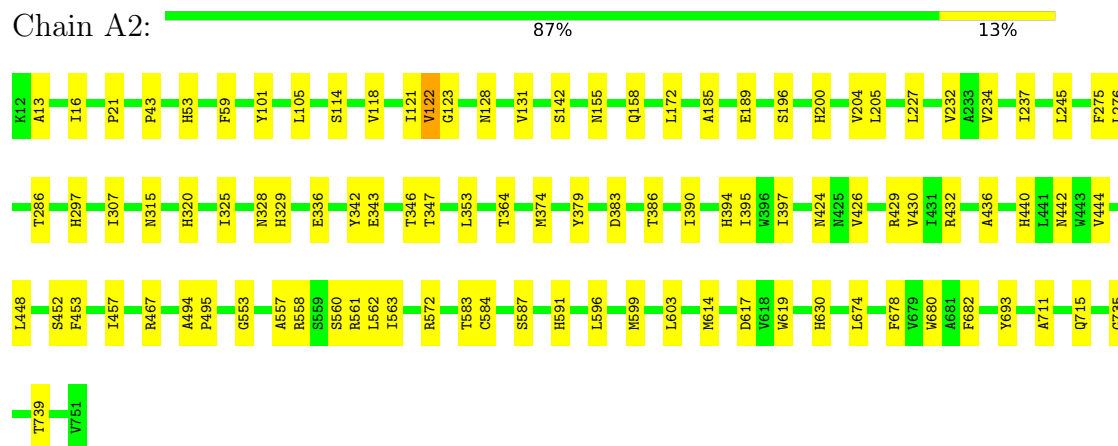
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

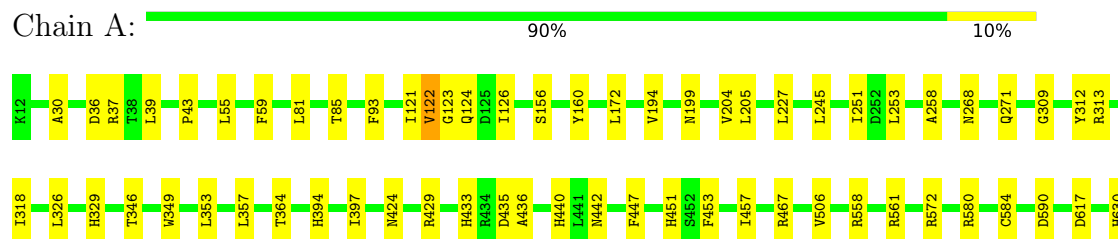
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

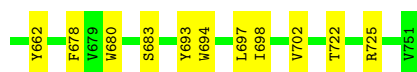


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



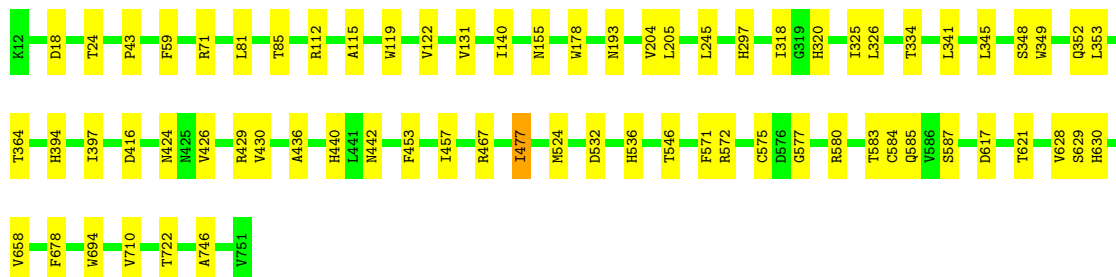
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1





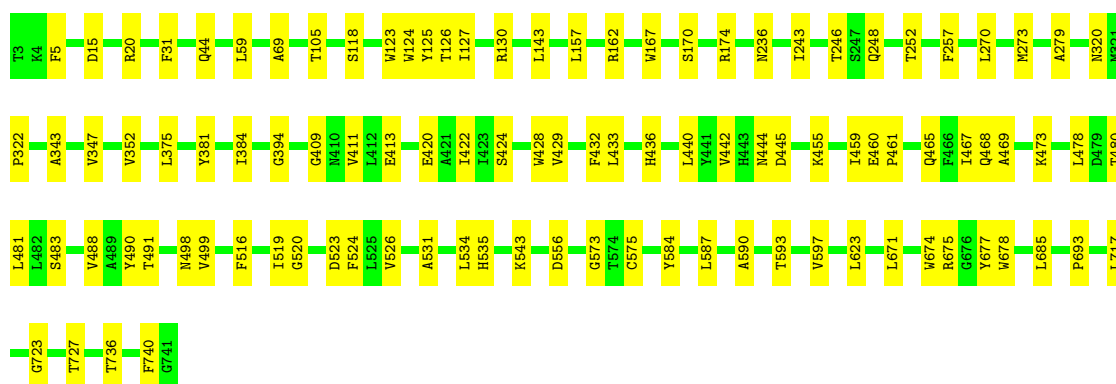
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain AA: 91% 9%



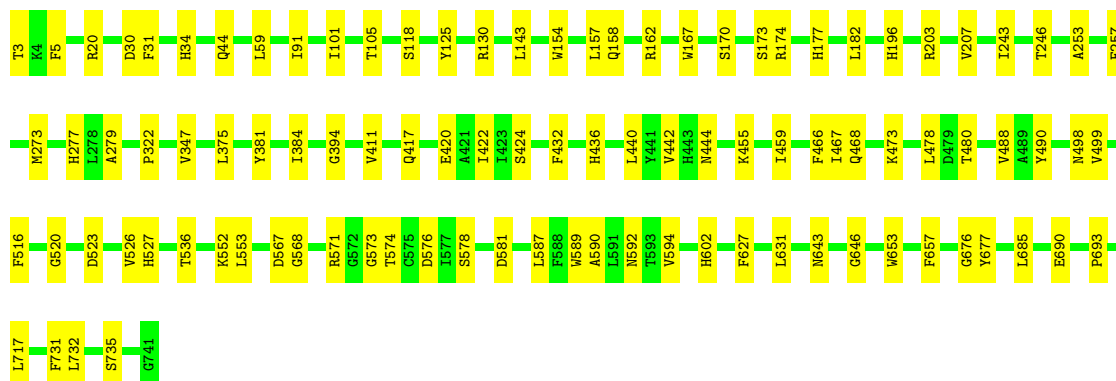
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1

Chain B1: 86% 14%



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1

Chain B2: 86% 14%



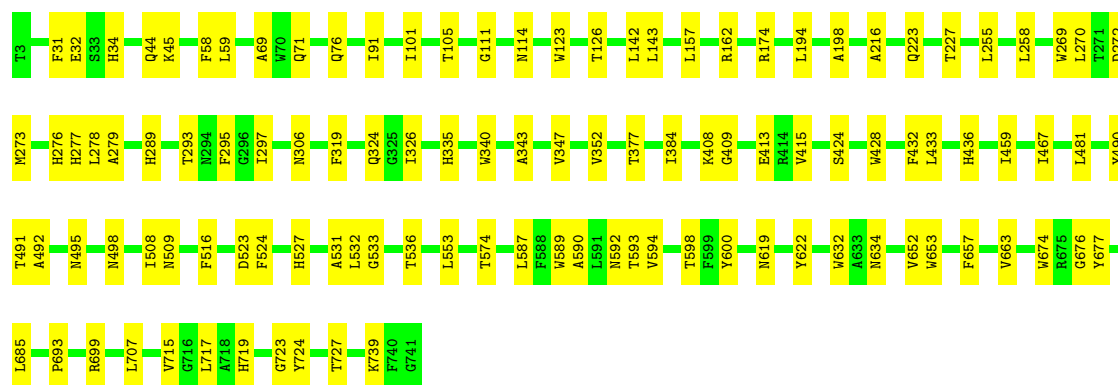
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1

Chain B: 87% 13%



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1

Chain BB: 85% 15%



- Molecule 3: Photosystem I iron-sulfur center

Chain C1: 84% 15%



- Molecule 3: Photosystem I iron-sulfur center

Chain C2: 88% 11%



- Molecule 3: Photosystem I iron-sulfur center

Chain C: 86% 14%



- Molecule 3: Photosystem I iron-sulfur center

Chain CC: 84% 16%



- Molecule 4: Photosystem I reaction center subunit II

Chain D1: 94% 6%



- Molecule 4: Photosystem I reaction center subunit II

Chain D2: 91% 9%



- Molecule 4: Photosystem I reaction center subunit II

Chain D: 93% 7%



- Molecule 4: Photosystem I reaction center subunit II

Chain DD: 94% 6%



- Molecule 5: Photosystem I reaction center subunit IV

Chain E1: 92% 8%



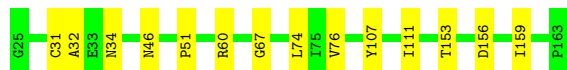
- Molecule 5: Photosystem I reaction center subunit IV

Chain E2: 92% 8%



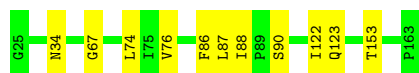
- Molecule 6: Photosystem I reaction center subunit III

Chain F1: 90% 10%




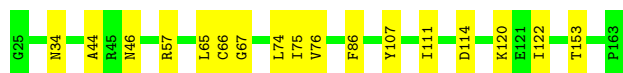
- Molecule 6: Photosystem I reaction center subunit III

Chain F:  92% 8%



- Molecule 6: Photosystem I reaction center subunit III

Chain FF:  88% 12%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain I1:  97%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain I:  94% 6%




- Molecule 7: Photosystem I reaction center subunit VIII

Chain II:  97%




- Molecule 8: Photosystem I reaction center subunit IX

Chain J1:  81% 8% 10%




- Molecule 8: Photosystem I reaction center subunit IX

Chain J2:  79% 10% 10%




- Molecule 8: Photosystem I reaction center subunit IX

Chain J:  83% 6% 10%



- Molecule 8: Photosystem I reaction center subunit IX

Chain JJ:  77% 13% 10%



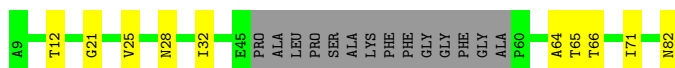
- Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain K1:  96%



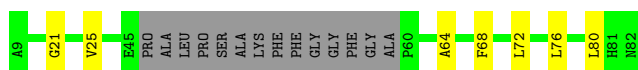
- Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain K:  68% 14% 19%




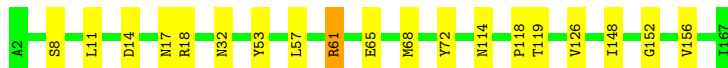
- Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain KK:  72% 9% 19%



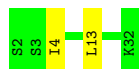
- Molecule 10: Photosystem I reaction center subunit XI

Chain L1:  89% 11%



- Molecule 11: Photosystem I reaction center subunit XII

Chain M1:  94% 6%



- Molecule 11: Photosystem I reaction center subunit XII

Chain M2:  97%



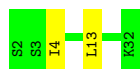
- Molecule 11: Photosystem I reaction center subunit XII

Chain M: 84% 16%



- Molecule 11: Photosystem I reaction center subunit XII

Chain MM: 94% 6%



- Molecule 12: Photosystem I 4.8 kDa protein

Chain X1: 92% 8%



- Molecule 12: Photosystem I 4.8 kDa protein

Chain X2: 90% 10%



- Molecule 12: Photosystem I 4.8 kDa protein

Chain X: 95% 5%



- Molecule 12: Photosystem I 4.8 kDa protein

Chain XX: 97% 3%

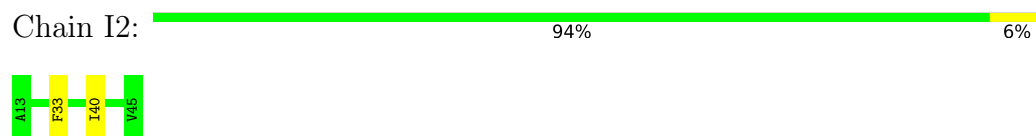


- Molecule 13: Photosystem I reaction center subunit III

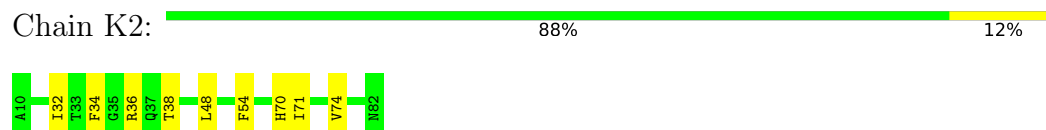
Chain F2: 85% 13% 2%



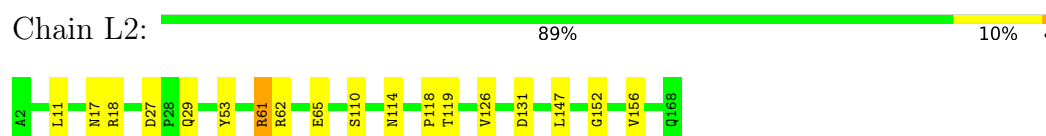
- Molecule 14: Photosystem I reaction center subunit VIII



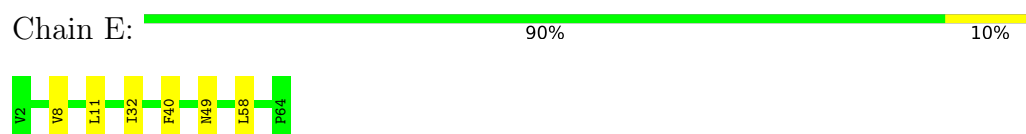
- Molecule 15: Photosystem I reaction center subunit PsaK 1



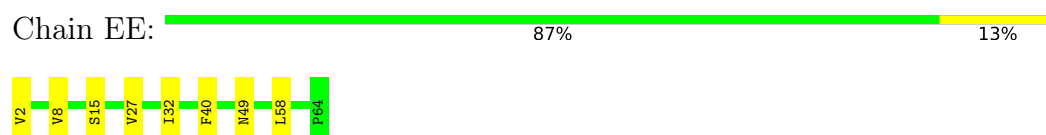
- Molecule 16: Photosystem I reaction center subunit XI



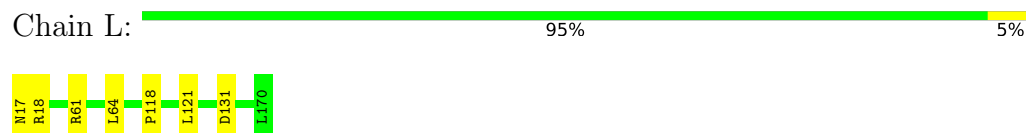
- Molecule 17: Photosystem I reaction center subunit IV



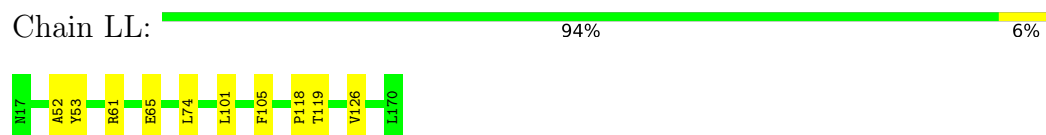
- Molecule 17: Photosystem I reaction center subunit IV



- Molecule 18: Photosystem I reaction center subunit XI



- Molecule 18: Photosystem I reaction center subunit XI



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	69247	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, DGD, AJP, SF4, CLA, PQN, ECH, CL0, BCR, LMG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	A	0.29	0/6004	0.44	0/8193
1	A1	0.28	0/6004	0.45	0/8193
1	A2	0.29	0/6004	0.46	0/8193
1	AA	0.28	0/6004	0.44	0/8193
10	L1	0.30	0/1281	0.46	0/1756
11	M	0.26	0/244	0.37	0/334
11	M1	0.26	0/244	0.42	0/334
11	M2	0.25	0/244	0.41	0/334
11	MM	0.26	0/244	0.39	0/334
12	X	0.29	0/320	0.46	0/439
12	X1	0.27	0/320	0.43	0/439
12	X2	0.29	0/320	0.44	0/439
12	XX	0.29	0/320	0.44	0/439
13	F2	0.29	0/1070	0.52	0/1455
14	I2	0.30	0/277	0.42	0/379
15	K2	0.26	0/546	0.45	0/748
16	L2	0.31	0/1290	0.47	0/1768
17	E	0.29	0/512	0.49	0/696
17	EE	0.28	0/512	0.48	0/696
18	L	0.30	0/1191	0.47	0/1632
18	LL	0.30	0/1191	0.45	0/1632
2	B	0.32	0/6143	0.46	0/8396
2	B1	0.29	0/6143	0.44	0/8396
2	B2	0.30	0/6143	0.44	0/8396
2	BB	0.32	0/6143	0.45	0/8396
3	C	0.28	0/609	0.52	0/826
3	C1	0.28	0/609	0.52	0/826
3	C2	0.28	0/609	0.49	0/826
3	CC	0.28	0/609	0.51	0/826
4	D	0.28	0/1060	0.52	0/1431
4	D1	0.27	0/1060	0.50	0/1431
4	D2	0.27	0/1060	0.53	0/1431

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
4	DD	0.28	0/1060	0.52	0/1431
5	E1	0.27	0/490	0.49	0/665
5	E2	0.30	0/490	0.47	0/665
6	F	0.28	0/1084	0.47	0/1475
6	F1	0.26	0/1084	0.46	0/1475
6	FF	0.27	0/1084	0.47	0/1475
7	I	0.29	0/262	0.41	0/358
7	I1	0.30	0/262	0.40	0/358
7	II	0.30	0/262	0.41	0/358
8	J	0.28	0/358	0.46	0/491
8	J1	0.27	0/358	0.43	0/491
8	J2	0.27	0/358	0.41	0/491
8	JJ	0.27	0/358	0.42	0/491
9	K	0.25	0/448	0.41	0/613
9	K1	0.27	0/551	0.45	0/755
9	KK	0.25	0/448	0.44	0/613
All	All	0.29	0/73287	0.46	0/100012

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
13	F2	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	F2	158	GLU	Peptide
13	F2	159	ILE	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5806	5677	5682	58	0
1	A1	5806	5672	5682	73	0
1	A2	5806	5680	5682	73	0
1	AA	5806	5677	5682	56	0
2	B	5919	5667	5677	73	0
2	B1	5919	5660	5677	82	0
2	B2	5919	5662	5677	79	0
2	BB	5919	5676	5677	89	0
3	C	599	582	585	8	0
3	C1	599	584	585	10	0
3	C2	599	580	585	6	0
3	CC	599	582	585	10	0
4	D	1036	1042	1042	9	0
4	D1	1036	1037	1042	7	0
4	D2	1036	1042	1042	10	0
4	DD	1036	1042	1042	7	0
5	E1	481	477	478	4	0
5	E2	481	477	478	7	0
6	F	1060	1051	1054	8	0
6	F1	1060	1052	1054	11	0
6	FF	1060	1052	1054	11	0
7	I	253	255	255	2	0
7	I1	253	255	255	1	0
7	II	253	255	255	1	0
8	J	346	355	355	3	0
8	J1	346	355	355	4	0
8	J2	346	355	355	5	0
8	JJ	346	354	355	5	0
9	K	439	461	461	6	0
9	K1	536	555	555	2	0
9	KK	439	461	461	4	0
10	L1	1244	1239	1242	16	0
11	M	240	256	256	5	0
11	M1	240	256	256	3	0
11	M2	240	256	256	1	0
11	MM	240	256	256	4	0
12	X	309	319	319	2	0
12	X1	309	318	319	4	0
12	X2	309	318	319	5	0
12	XX	309	319	319	1	0
13	F2	1047	1040	1042	15	0
14	I2	268	268	268	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	K2	531	550	550	7	0
16	L2	1253	1245	1250	12	0
17	E	502	492	496	5	0
17	EE	502	492	496	6	0
18	L	1156	1153	1157	4	0
18	LL	1156	1154	1157	8	0
19	A	2339	2207	2215	48	0
19	A1	2394	2261	2275	59	0
19	A2	2375	2227	2236	47	0
19	AA	2404	2279	2287	43	0
19	B	2401	2357	2375	73	0
19	B1	2291	2253	2270	61	0
19	B2	2401	2358	2375	50	0
19	BB	2271	2219	2231	64	0
19	F	102	89	90	3	0
19	F1	147	122	123	5	0
19	F2	102	89	90	3	0
19	FF	167	161	162	6	0
19	J	82	58	58	4	0
19	J1	82	57	58	1	0
19	J2	82	58	58	2	0
19	JJ	82	57	58	1	0
19	K	91	65	66	0	0
19	K1	131	92	94	2	0
19	K2	86	61	62	1	0
19	KK	91	65	66	0	0
19	L	191	198	205	4	0
19	L1	191	202	205	5	0
19	L2	186	187	191	0	0
19	LL	168	155	164	7	0
19	X	45	32	33	0	0
19	X1	45	32	33	0	0
19	X2	45	32	33	1	0
19	XX	45	32	33	0	0
20	A	65	72	72	1	0
20	A1	65	72	71	3	0
20	A2	65	72	70	5	0
20	AA	65	72	71	1	0
21	A	33	46	46	3	0
21	A1	33	46	46	1	0
21	A2	33	46	46	1	0
21	AA	33	46	46	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	B	33	46	46	2	0
21	B1	33	46	46	0	0
21	B2	33	46	46	0	0
21	BB	33	46	46	2	0
22	A	87	122	123	3	0
22	A1	87	122	123	1	0
22	A2	87	122	123	2	0
22	AA	87	122	123	3	0
22	B	82	110	110	1	0
22	B1	33	36	36	1	0
22	B2	33	36	36	0	0
22	BB	82	110	110	0	0
22	L	34	42	38	0	0
22	L1	33	35	36	3	0
22	L2	35	39	40	2	0
22	LL	34	42	38	0	0
22	X	40	49	50	0	0
22	X1	89	123	124	0	0
22	X2	89	123	124	0	0
22	XX	40	49	50	0	0
23	A	279	389	389	7	0
23	A1	239	333	333	6	0
23	A2	239	333	333	7	0
23	AA	279	389	389	8	0
23	B	240	336	336	12	0
23	B1	200	280	280	7	0
23	B2	200	275	280	8	0
23	BB	240	336	336	10	0
23	F	120	163	168	8	0
23	F1	120	163	168	7	0
23	F2	120	163	168	7	0
23	FF	120	163	168	7	0
23	I	80	112	112	0	0
23	I1	40	56	56	1	0
23	I2	120	168	168	1	0
23	II	120	168	168	0	0
23	J	80	112	112	2	0
23	J1	80	112	112	2	0
23	J2	80	112	112	3	0
23	JJ	80	112	112	2	0
23	K	40	56	56	0	0
23	K1	80	112	112	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	K2	80	112	112	3	0
23	KK	40	56	56	0	0
23	L	80	112	112	1	0
23	L1	120	168	168	0	0
23	L2	40	56	56	0	0
23	LL	40	56	56	1	0
23	M	40	51	56	2	0
23	M1	40	56	56	0	0
23	M2	40	56	56	0	0
23	MM	40	53	56	1	0
24	A	65	88	0	0	0
24	A1	75	96	0	0	0
24	A2	32	43	0	0	0
24	AA	65	88	0	0	0
24	B	129	159	0	1	0
24	BB	86	106	0	1	0
24	I2	31	42	0	0	0
24	K	41	50	0	0	0
24	KK	41	50	0	0	0
24	L	62	85	0	0	0
24	L1	86	106	0	1	0
24	L2	86	106	0	1	0
24	M2	31	43	0	0	0
25	A1	68	84	0	0	0
25	A2	74	97	0	0	0
25	B	176	251	172	0	0
25	B1	117	148	150	0	0
25	B2	117	148	150	0	0
25	BB	122	167	86	0	0
25	I1	35	40	40	0	0
25	I2	35	40	40	1	0
25	II	79	102	54	0	0
25	K1	58	62	0	0	0
25	K2	56	58	0	0	0
25	L	37	48	0	0	0
25	L1	91	132	86	1	0
25	L2	36	46	0	0	0
25	M	46	59	62	1	0
26	B	41	54	54	1	0
26	B1	41	54	54	1	0
26	B2	41	54	54	1	0
26	BB	41	54	54	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	B	8	0	0	0	0
27	B1	8	0	0	0	0
27	B2	8	0	0	0	0
27	BB	8	0	0	0	0
27	C	16	0	0	1	0
27	C1	16	0	0	1	0
27	C2	16	0	0	0	0
27	CC	16	0	0	0	0
28	B	42	46	42	1	0
28	BB	42	46	42	1	0
All	All	99604	99577	98156	1039	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 1039 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B2:587:LEU:HD23	2:B2:717:LEU:HD21	1.55	0.88
2:B:553:LEU:HD23	2:B:577:ILE:HD11	1.56	0.86
19:B2:822:CLA:H93	23:B2:843:BCR:H333	1.57	0.84
19:B1:822:CLA:H93	23:B1:842:BCR:H333	1.58	0.83
2:B1:534:LEU:HD12	19:B1:834:CLA:HED3	1.63	0.81

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	738/740 (100%)	713 (97%)	24 (3%)	1 (0%)	53	87
1	A1	738/740 (100%)	710 (96%)	27 (4%)	1 (0%)	53	87

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A2	738/740 (100%)	714 (97%)	23 (3%)	1 (0%)	53	87
1	AA	738/740 (100%)	709 (96%)	28 (4%)	1 (0%)	53	87
2	B	737/739 (100%)	712 (97%)	25 (3%)	0	100	100
2	B1	737/739 (100%)	715 (97%)	22 (3%)	0	100	100
2	B2	737/739 (100%)	713 (97%)	24 (3%)	0	100	100
2	BB	737/739 (100%)	710 (96%)	27 (4%)	0	100	100
3	C	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
3	C1	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
3	C2	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
3	CC	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
4	D	132/134 (98%)	122 (92%)	10 (8%)	0	100	100
4	D1	132/134 (98%)	121 (92%)	11 (8%)	0	100	100
4	D2	132/134 (98%)	125 (95%)	7 (5%)	0	100	100
4	DD	132/134 (98%)	125 (95%)	7 (5%)	0	100	100
5	E1	58/60 (97%)	56 (97%)	2 (3%)	0	100	100
5	E2	58/60 (97%)	54 (93%)	4 (7%)	0	100	100
6	F	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
6	F1	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
6	FF	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
7	I	29/31 (94%)	29 (100%)	0	0	100	100
7	I1	29/31 (94%)	29 (100%)	0	0	100	100
7	II	29/31 (94%)	29 (100%)	0	0	100	100
8	J	41/48 (85%)	40 (98%)	1 (2%)	0	100	100
8	J1	41/48 (85%)	38 (93%)	3 (7%)	0	100	100
8	J2	41/48 (85%)	39 (95%)	2 (5%)	0	100	100
8	JJ	41/48 (85%)	38 (93%)	3 (7%)	0	100	100
9	K	56/74 (76%)	55 (98%)	1 (2%)	0	100	100
9	K1	72/74 (97%)	71 (99%)	1 (1%)	0	100	100
9	KK	56/74 (76%)	55 (98%)	1 (2%)	0	100	100
10	L1	164/166 (99%)	160 (98%)	4 (2%)	0	100	100
11	M	29/31 (94%)	29 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	M1	29/31 (94%)	29 (100%)	0	0	100	100
11	M2	29/31 (94%)	29 (100%)	0	0	100	100
11	MM	29/31 (94%)	29 (100%)	0	0	100	100
12	X	37/39 (95%)	35 (95%)	2 (5%)	0	100	100
12	X1	37/39 (95%)	35 (95%)	2 (5%)	0	100	100
12	X2	37/39 (95%)	35 (95%)	2 (5%)	0	100	100
12	XX	37/39 (95%)	35 (95%)	2 (5%)	0	100	100
13	F2	135/137 (98%)	125 (93%)	7 (5%)	3 (2%)	7	39
14	I2	31/33 (94%)	31 (100%)	0	0	100	100
15	K2	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
16	L2	165/167 (99%)	160 (97%)	5 (3%)	0	100	100
17	E	61/63 (97%)	61 (100%)	0	0	100	100
17	EE	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
18	L	152/154 (99%)	146 (96%)	5 (3%)	1 (1%)	24	66
18	LL	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
All	All	8958/9106 (98%)	8634 (96%)	316 (4%)	8 (0%)	56	87

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A2	122	VAL
13	F2	159	ILE
1	A1	122	VAL
1	A	122	VAL
1	AA	477	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	594/594 (100%)	594 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A1	594/594 (100%)	594 (100%)	0	100	100
1	A2	594/594 (100%)	594 (100%)	0	100	100
1	AA	594/594 (100%)	594 (100%)	0	100	100
2	B	601/601 (100%)	601 (100%)	0	100	100
2	B1	601/601 (100%)	601 (100%)	0	100	100
2	B2	601/601 (100%)	601 (100%)	0	100	100
2	BB	601/601 (100%)	600 (100%)	1 (0%)	94	98
3	C	68/68 (100%)	68 (100%)	0	100	100
3	C1	68/68 (100%)	67 (98%)	1 (2%)	67	88
3	C2	68/68 (100%)	67 (98%)	1 (2%)	67	88
3	CC	68/68 (100%)	68 (100%)	0	100	100
4	D	107/107 (100%)	107 (100%)	0	100	100
4	D1	107/107 (100%)	107 (100%)	0	100	100
4	D2	107/107 (100%)	107 (100%)	0	100	100
4	DD	107/107 (100%)	107 (100%)	0	100	100
5	E1	53/53 (100%)	53 (100%)	0	100	100
5	E2	53/53 (100%)	53 (100%)	0	100	100
6	F	108/108 (100%)	108 (100%)	0	100	100
6	F1	108/108 (100%)	108 (100%)	0	100	100
6	FF	108/108 (100%)	108 (100%)	0	100	100
7	I	28/28 (100%)	28 (100%)	0	100	100
7	I1	28/28 (100%)	28 (100%)	0	100	100
7	II	28/28 (100%)	28 (100%)	0	100	100
8	J	38/41 (93%)	38 (100%)	0	100	100
8	J1	38/41 (93%)	38 (100%)	0	100	100
8	J2	38/41 (93%)	38 (100%)	0	100	100
8	JJ	38/41 (93%)	38 (100%)	0	100	100
9	K	46/54 (85%)	46 (100%)	0	100	100
9	K1	54/54 (100%)	54 (100%)	0	100	100
9	KK	46/54 (85%)	46 (100%)	0	100	100
10	L1	127/127 (100%)	126 (99%)	1 (1%)	83	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	M	26/26 (100%)	26 (100%)	0	100	100
11	M1	26/26 (100%)	26 (100%)	0	100	100
11	M2	26/26 (100%)	26 (100%)	0	100	100
11	MM	26/26 (100%)	26 (100%)	0	100	100
12	X	31/31 (100%)	31 (100%)	0	100	100
12	X1	31/31 (100%)	31 (100%)	0	100	100
12	X2	31/31 (100%)	31 (100%)	0	100	100
12	XX	31/31 (100%)	31 (100%)	0	100	100
13	F2	106/106 (100%)	106 (100%)	0	100	100
14	I2	30/30 (100%)	30 (100%)	0	100	100
15	K2	54/54 (100%)	54 (100%)	0	100	100
16	L2	128/128 (100%)	127 (99%)	1 (1%)	83	94
17	E	55/55 (100%)	55 (100%)	0	100	100
17	EE	55/55 (100%)	55 (100%)	0	100	100
18	L	117/117 (100%)	116 (99%)	1 (1%)	81	93
18	LL	117/117 (100%)	117 (100%)	0	100	100
All	All	7309/7337 (100%)	7303 (100%)	6 (0%)	94	98

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C2	44	ARG
2	BB	34	HIS
16	L2	61	ARG
10	L1	61	ARG
18	L	61	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
2	B2	341	HIS
5	E2	19	GLN
2	BB	223	GLN
2	B2	610	GLN
16	L2	114	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

594 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
19	CLA	A	801	-	57,73,73	1.04	5 (8%)	66,113,113	1.48	9 (13%)
24	AJP	A	802	-	35,35,95	4.43	22 (62%)	52,58,149	4.37	28 (53%)
20	CL0	A	803	-	57,73,73	1.85	11 (19%)	66,113,113	2.32	21 (31%)
19	CLA	A	804	-	57,73,73	1.06	4 (7%)	66,113,113	1.46	9 (13%)
19	CLA	A	805	-	52,68,73	1.08	4 (7%)	60,107,113	1.56	9 (15%)
19	CLA	A	806	-	48,64,73	1.14	6 (12%)	55,102,113	1.69	12 (21%)
19	CLA	A	807	-	57,73,73	1.06	5 (8%)	66,113,113	1.34	8 (12%)
19	CLA	A	808	-	57,73,73	1.04	4 (7%)	66,113,113	1.47	10 (15%)
19	CLA	A	809	-	42,58,73	1.19	4 (9%)	48,95,113	1.65	10 (20%)
19	CLA	A	810	1	57,73,73	1.02	5 (8%)	66,113,113	1.57	12 (18%)
19	CLA	A	811	1	43,59,73	1.24	7 (16%)	49,96,113	1.67	9 (18%)
19	CLA	A	812	-	38,54,73	1.23	4 (10%)	43,90,113	1.72	8 (18%)
19	CLA	A	813	-	57,73,73	1.02	4 (7%)	66,113,113	1.44	9 (13%)
19	CLA	A	814	-	34,50,73	1.28	4 (11%)	38,85,113	1.66	7 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A	815	-	47,63,73	1.13	4 (8%)	54,101,113	1.54	8 (14%)
19	CLA	A	816	-	42,58,73	1.20	4 (9%)	48,95,113	1.60	9 (18%)
19	CLA	A	817	-	36,52,73	1.24	4 (11%)	39,87,113	1.72	8 (20%)
19	CLA	A	818	-	34,53,73	1.28	4 (11%)	37,89,113	1.70	6 (16%)
19	CLA	A	819	-	52,68,73	1.08	5 (9%)	60,107,113	1.51	9 (15%)
19	CLA	A	820	-	50,66,73	1.16	7 (14%)	57,104,113	1.58	11 (19%)
19	CLA	A	821	-	57,73,73	1.00	5 (8%)	66,113,113	1.54	11 (16%)
19	CLA	A	822	-	43,59,73	1.19	4 (9%)	49,96,113	1.58	7 (14%)
19	CLA	A	823	-	52,68,73	1.09	5 (9%)	60,107,113	1.62	10 (16%)
19	CLA	A	824	-	34,53,73	1.26	4 (11%)	37,89,113	1.82	8 (21%)
19	CLA	A	825	-	44,60,73	1.16	4 (9%)	50,97,113	1.59	8 (16%)
19	CLA	A	826	-	34,53,73	1.28	5 (14%)	37,89,113	1.72	8 (21%)
19	CLA	A	827	-	57,73,73	1.05	6 (10%)	66,113,113	1.34	4 (6%)
19	CLA	A	828	-	48,64,73	1.11	4 (8%)	55,102,113	1.56	8 (14%)
19	CLA	A	829	-	57,73,73	1.03	5 (8%)	66,113,113	1.49	9 (13%)
19	CLA	A	830	-	54,70,73	1.01	5 (9%)	62,109,113	1.50	9 (14%)
19	CLA	A	831	-	57,73,73	1.05	4 (7%)	66,113,113	1.41	8 (12%)
19	CLA	A	832	-	57,73,73	1.01	5 (8%)	66,113,113	1.51	11 (16%)
19	CLA	A	833	-	42,58,73	1.20	6 (14%)	48,95,113	1.52	6 (12%)
19	CLA	A	834	-	33,49,73	1.31	5 (15%)	37,84,113	1.74	8 (21%)
19	CLA	A	835	-	57,73,73	1.06	4 (7%)	66,113,113	1.41	9 (13%)
19	CLA	A	836	-	57,73,73	1.03	6 (10%)	66,113,113	1.44	7 (10%)
19	CLA	A	837	-	34,53,73	1.31	4 (11%)	37,89,113	1.74	8 (21%)
19	CLA	A	838	-	36,52,73	1.25	4 (11%)	39,87,113	1.81	8 (20%)
19	CLA	A	839	-	44,60,73	1.16	4 (9%)	50,97,113	1.62	9 (18%)
19	CLA	A	840	-	48,64,73	1.12	5 (10%)	55,102,113	1.54	8 (14%)
19	CLA	A	841	-	38,54,73	1.21	4 (10%)	43,90,113	1.71	8 (18%)
19	CLA	A	842	-	57,73,73	1.04	6 (10%)	66,113,113	1.53	12 (18%)
21	PQN	A	843	-	34,34,34	0.59	0	42,45,45	1.07	3 (7%)
19	CLA	A	844	-	33,49,73	1.30	4 (12%)	37,84,113	1.81	7 (18%)
22	LHG	A	845	-	48,48,48	0.79	2 (4%)	51,54,54	0.97	3 (5%)
22	LHG	A	846	-	37,37,48	0.81	1 (2%)	40,43,54	1.01	3 (7%)
23	BCR	A	847	-	40,40,41	1.09	2 (5%)	53,54,56	1.26	9 (16%)
23	BCR	A	848	-	41,41,41	1.14	2 (4%)	56,56,56	1.22	8 (14%)
23	BCR	A	849	-	41,41,41	1.07	2 (4%)	56,56,56	1.26	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCR	A	850	-	41,41,41	1.13	2 (4%)	56,56,56	1.23	4 (7%)
23	BCR	A	851	-	41,41,41	1.06	1 (2%)	56,56,56	1.46	8 (14%)
19	CLA	A	852	-	57,73,73	1.07	7 (12%)	66,113,113	1.45	10 (15%)
23	BCR	A	853	-	41,41,41	1.13	2 (4%)	56,56,56	1.35	10 (17%)
23	BCR	A	854	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	8 (14%)
24	AJP	A	855	-	40,40,95	4.24	24 (60%)	57,65,149	3.45	19 (33%)
19	CLA	A1	801	-	57,73,73	1.04	5 (8%)	66,113,113	1.51	10 (15%)
20	CL0	A1	802	-	57,73,73	1.87	12 (21%)	66,113,113	2.27	23 (34%)
19	CLA	A1	803	-	57,73,73	1.03	4 (7%)	66,113,113	1.46	9 (13%)
19	CLA	A1	804	-	52,68,73	1.07	4 (7%)	60,107,113	1.43	9 (15%)
19	CLA	A1	805	-	48,64,73	1.15	7 (14%)	55,102,113	1.52	8 (14%)
19	CLA	A1	806	-	57,73,73	1.06	6 (10%)	66,113,113	1.39	8 (12%)
19	CLA	A1	807	-	57,73,73	1.04	4 (7%)	66,113,113	1.48	8 (12%)
19	CLA	A1	808	-	42,58,73	1.19	4 (9%)	48,95,113	1.70	9 (18%)
19	CLA	A1	809	-	57,73,73	1.02	5 (8%)	66,113,113	1.49	12 (18%)
19	CLA	A1	810	-	43,59,73	1.22	7 (16%)	49,96,113	1.68	9 (18%)
19	CLA	A1	811	-	38,54,73	1.24	4 (10%)	43,90,113	1.69	9 (20%)
19	CLA	A1	812	-	57,73,73	1.02	4 (7%)	66,113,113	1.44	9 (13%)
19	CLA	A1	813	-	34,50,73	1.26	4 (11%)	38,85,113	1.70	8 (21%)
19	CLA	A1	814	-	47,63,73	1.12	4 (8%)	54,101,113	1.54	8 (14%)
19	CLA	A1	815	-	42,58,73	1.19	4 (9%)	48,95,113	1.62	9 (18%)
19	CLA	A1	816	-	36,52,73	1.26	5 (13%)	39,87,113	1.71	8 (20%)
19	CLA	A1	817	-	34,53,73	1.29	4 (11%)	37,89,113	1.73	8 (21%)
19	CLA	A1	818	-	52,68,73	1.09	4 (7%)	60,107,113	1.50	8 (13%)
19	CLA	A1	819	-	50,66,73	1.17	7 (14%)	57,104,113	1.55	10 (17%)
19	CLA	A1	820	-	57,73,73	0.99	5 (8%)	66,113,113	1.55	12 (18%)
19	CLA	A1	821	-	43,59,73	1.19	4 (9%)	49,96,113	1.61	9 (18%)
19	CLA	A1	822	-	52,68,73	1.09	6 (11%)	60,107,113	1.57	10 (16%)
19	CLA	A1	823	-	34,53,73	1.28	4 (11%)	37,89,113	1.84	8 (21%)
19	CLA	A1	824	-	34,50,73	1.32	5 (14%)	38,85,113	1.69	8 (21%)
19	CLA	A1	825	-	34,53,73	1.28	4 (11%)	37,89,113	1.77	7 (18%)
19	CLA	A1	826	-	57,73,73	1.06	6 (10%)	66,113,113	1.42	5 (7%)
19	CLA	A1	827	-	48,64,73	1.13	4 (8%)	55,102,113	1.57	9 (16%)
19	CLA	A1	828	-	57,73,73	1.02	4 (7%)	66,113,113	1.49	10 (15%)
19	CLA	A1	829	-	54,70,73	1.03	4 (7%)	62,109,113	1.46	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A1	830	-	57,73,73	1.05	4 (7%)	66,113,113	1.40	10 (15%)
19	CLA	A1	831	-	57,73,73	1.01	5 (8%)	66,113,113	1.49	8 (12%)
19	CLA	A1	832	-	42,58,73	1.21	6 (14%)	48,95,113	1.55	7 (14%)
19	CLA	A1	833	-	33,49,73	1.31	5 (15%)	37,84,113	1.76	8 (21%)
19	CLA	A1	834	-	57,73,73	1.06	6 (10%)	66,113,113	1.41	10 (15%)
19	CLA	A1	835	-	57,73,73	1.04	6 (10%)	66,113,113	1.43	7 (10%)
19	CLA	A1	836	-	34,53,73	1.32	5 (14%)	37,89,113	1.75	8 (21%)
19	CLA	A1	837	1	36,52,73	1.24	4 (11%)	39,87,113	1.86	9 (23%)
19	CLA	A1	838	-	44,60,73	1.17	4 (9%)	50,97,113	1.64	7 (14%)
19	CLA	A1	839	-	48,64,73	1.12	4 (8%)	55,102,113	1.49	7 (12%)
19	CLA	A1	840	-	38,54,73	1.23	4 (10%)	43,90,113	1.70	7 (16%)
19	CLA	A1	841	-	57,73,73	1.03	6 (10%)	66,113,113	1.52	9 (13%)
19	CLA	A1	842	-	57,73,73	1.08	6 (10%)	66,113,113	1.70	12 (18%)
21	PQN	A1	843	-	34,34,34	0.62	0	42,45,45	1.07	3 (7%)
19	CLA	A1	844	-	33,49,73	1.30	4 (12%)	37,84,113	1.78	7 (18%)
22	LHG	A1	845	-	48,48,48	0.77	2 (4%)	51,54,54	0.95	3 (5%)
22	LHG	A1	846	-	37,37,48	0.81	1 (2%)	40,43,54	1.00	3 (7%)
23	BCR	A1	847	-	40,40,41	1.10	2 (5%)	53,54,56	1.24	7 (13%)
23	BCR	A1	848	-	41,41,41	1.14	2 (4%)	56,56,56	1.22	6 (10%)
23	BCR	A1	849	-	41,41,41	1.08	2 (4%)	56,56,56	1.25	7 (12%)
23	BCR	A1	850	-	41,41,41	1.17	2 (4%)	56,56,56	1.26	6 (10%)
23	BCR	A1	851	-	41,41,41	1.07	1 (2%)	56,56,56	1.47	8 (14%)
19	CLA	A1	852	-	57,73,73	1.05	6 (10%)	66,113,113	1.41	7 (10%)
23	BCR	A1	853	-	41,41,41	1.12	2 (4%)	56,56,56	1.36	9 (16%)
24	AJP	A1	854	-	49,49,95	3.88	25 (51%)	71,80,149	3.22	19 (26%)
24	AJP	A1	855	-	37,37,95	4.35	24 (64%)	56,62,149	3.41	21 (37%)
19	CLA	A2	801	-	57,73,73	1.03	5 (8%)	66,113,113	1.49	8 (12%)
19	CLA	A2	802	-	38,54,73	1.22	4 (10%)	43,90,113	1.69	7 (16%)
20	CL0	A2	803	-	57,73,73	1.79	12 (21%)	66,113,113	2.39	20 (30%)
19	CLA	A2	804	-	57,73,73	1.03	5 (8%)	66,113,113	1.44	9 (13%)
19	CLA	A2	805	-	52,68,73	1.07	4 (7%)	60,107,113	1.54	10 (16%)
19	CLA	A2	806	-	48,64,73	1.14	7 (14%)	55,102,113	1.68	10 (18%)
19	CLA	A2	807	-	57,73,73	1.06	5 (8%)	66,113,113	1.39	8 (12%)
19	CLA	A2	808	-	57,73,73	1.02	5 (8%)	66,113,113	1.42	8 (12%)
19	CLA	A2	809	-	42,58,73	1.19	4 (9%)	48,95,113	1.68	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A2	810	1	57,73,73	1.03	5 (8%)	66,113,113	1.54	12 (18%)
19	CLA	A2	811	-	43,59,73	1.22	7 (16%)	49,96,113	1.69	9 (18%)
19	CLA	A2	812	-	38,54,73	1.23	5 (13%)	43,90,113	1.68	10 (23%)
19	CLA	A2	813	-	57,73,73	1.02	4 (7%)	66,113,113	1.47	9 (13%)
19	CLA	A2	814	-	34,50,73	1.27	4 (11%)	38,85,113	1.69	7 (18%)
19	CLA	A2	815	-	47,63,73	1.12	4 (8%)	54,101,113	1.50	8 (14%)
19	CLA	A2	816	-	42,58,73	1.19	4 (9%)	48,95,113	1.62	9 (18%)
19	CLA	A2	817	-	36,52,73	1.26	4 (11%)	39,87,113	1.72	8 (20%)
19	CLA	A2	818	-	34,53,73	1.30	4 (11%)	37,89,113	1.72	8 (21%)
19	CLA	A2	819	-	52,68,73	1.09	5 (9%)	60,107,113	1.49	8 (13%)
19	CLA	A2	820	-	50,66,73	1.17	7 (14%)	57,104,113	1.58	10 (17%)
19	CLA	A2	821	-	57,73,73	0.99	5 (8%)	66,113,113	1.49	10 (15%)
19	CLA	A2	822	-	43,59,73	1.19	4 (9%)	49,96,113	1.62	8 (16%)
19	CLA	A2	823	-	52,68,73	1.09	5 (9%)	60,107,113	1.67	11 (18%)
19	CLA	A2	824	-	34,53,73	1.28	4 (11%)	37,89,113	1.81	8 (21%)
19	CLA	A2	825	-	34,50,73	1.32	6 (17%)	38,85,113	1.76	8 (21%)
19	CLA	A2	826	-	34,53,73	1.29	6 (17%)	37,89,113	1.77	7 (18%)
19	CLA	A2	827	-	57,73,73	1.06	6 (10%)	66,113,113	1.49	8 (12%)
19	CLA	A2	828	-	48,64,73	1.12	4 (8%)	55,102,113	1.58	8 (14%)
19	CLA	A2	829	-	57,73,73	1.06	7 (12%)	66,113,113	1.42	11 (16%)
19	CLA	A2	830	-	54,70,73	1.04	4 (7%)	62,109,113	1.48	10 (16%)
19	CLA	A2	831	-	57,73,73	1.06	6 (10%)	66,113,113	1.39	8 (12%)
19	CLA	A2	832	-	57,73,73	1.02	5 (8%)	66,113,113	1.51	9 (13%)
19	CLA	A2	833	-	42,58,73	1.21	6 (14%)	48,95,113	1.49	8 (16%)
19	CLA	A2	834	-	33,49,73	1.31	5 (15%)	37,84,113	1.77	10 (27%)
19	CLA	A2	835	-	57,73,73	1.07	6 (10%)	66,113,113	1.44	10 (15%)
19	CLA	A2	836	-	57,73,73	1.06	6 (10%)	66,113,113	1.54	9 (13%)
19	CLA	A2	837	-	34,53,73	1.33	5 (14%)	37,89,113	1.77	8 (21%)
19	CLA	A2	838	-	36,52,73	1.24	4 (11%)	39,87,113	1.85	9 (23%)
19	CLA	A2	839	-	44,60,73	1.16	4 (9%)	50,97,113	1.62	8 (16%)
19	CLA	A2	840	-	48,64,73	1.11	4 (8%)	55,102,113	1.52	7 (12%)
19	CLA	A2	841	-	38,54,73	1.22	4 (10%)	43,90,113	1.71	7 (16%)
19	CLA	A2	842	-	57,73,73	1.04	6 (10%)	66,113,113	1.57	10 (15%)
21	PQN	A2	843	-	34,34,34	0.62	0	42,45,45	1.07	3 (7%)
19	CLA	A2	844	-	33,49,73	1.30	5 (15%)	37,84,113	1.77	7 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	LHG	A2	845	-	48,48,48	0.76	1 (2%)	51,54,54	0.95	3 (5%)
22	LHG	A2	846	-	37,37,48	0.81	1 (2%)	40,43,54	1.01	3 (7%)
23	BCR	A2	847	-	40,40,41	1.09	2 (5%)	53,54,56	1.24	7 (13%)
23	BCR	A2	848	-	41,41,41	1.14	2 (4%)	56,56,56	1.23	6 (10%)
23	BCR	A2	849	-	41,41,41	1.04	2 (4%)	56,56,56	1.25	8 (14%)
23	BCR	A2	850	-	41,41,41	1.16	2 (4%)	56,56,56	1.23	6 (10%)
23	BCR	A2	851	-	41,41,41	1.06	1 (2%)	56,56,56	1.48	10 (17%)
19	CLA	A2	852	-	57,73,73	1.08	6 (10%)	66,113,113	1.49	8 (12%)
23	BCR	A2	853	-	41,41,41	1.12	2 (4%)	56,56,56	1.36	8 (14%)
24	AJP	A2	854	-	37,37,95	4.35	24 (64%)	56,62,149	3.42	20 (35%)
19	CLA	AA	801	-	57,73,73	1.04	7 (12%)	66,113,113	1.45	7 (10%)
24	AJP	AA	802	-	35,35,95	4.43	22 (62%)	52,58,149	4.37	28 (53%)
20	CL0	AA	803	-	57,73,73	1.84	12 (21%)	66,113,113	2.42	20 (30%)
19	CLA	AA	804	-	57,73,73	1.05	4 (7%)	66,113,113	1.46	9 (13%)
19	CLA	AA	805	-	52,68,73	1.07	4 (7%)	60,107,113	1.57	10 (16%)
19	CLA	AA	806	-	48,64,73	1.15	6 (12%)	55,102,113	1.68	11 (20%)
19	CLA	AA	807	-	57,73,73	1.05	5 (8%)	66,113,113	1.33	6 (9%)
19	CLA	AA	808	-	57,73,73	1.02	4 (7%)	66,113,113	1.40	8 (12%)
19	CLA	AA	809	-	42,58,73	1.19	4 (9%)	48,95,113	1.66	9 (18%)
19	CLA	AA	810	-	57,73,73	1.03	5 (8%)	66,113,113	1.56	13 (19%)
19	CLA	AA	811	1	43,59,73	1.23	6 (13%)	49,96,113	1.69	8 (16%)
19	CLA	AA	812	-	38,54,73	1.24	4 (10%)	43,90,113	1.71	8 (18%)
19	CLA	AA	813	-	57,73,73	1.02	4 (7%)	66,113,113	1.45	9 (13%)
19	CLA	AA	814	-	34,50,73	1.28	4 (11%)	38,85,113	1.70	8 (21%)
19	CLA	AA	815	-	47,63,73	1.13	4 (8%)	54,101,113	1.53	7 (12%)
19	CLA	AA	816	-	42,58,73	1.21	5 (11%)	48,95,113	1.61	10 (20%)
19	CLA	AA	817	-	36,52,73	1.25	4 (11%)	39,87,113	1.71	8 (20%)
19	CLA	AA	818	-	34,53,73	1.28	4 (11%)	37,89,113	1.72	7 (18%)
19	CLA	AA	819	-	52,68,73	1.09	4 (7%)	60,107,113	1.48	9 (15%)
19	CLA	AA	820	-	50,66,73	1.15	7 (14%)	57,104,113	1.58	10 (17%)
19	CLA	AA	821	-	57,73,73	1.00	5 (8%)	66,113,113	1.49	9 (13%)
19	CLA	AA	822	-	43,59,73	1.18	4 (9%)	49,96,113	1.59	8 (16%)
19	CLA	AA	823	-	52,68,73	1.09	5 (9%)	60,107,113	1.61	10 (16%)
19	CLA	AA	824	-	34,53,73	1.27	4 (11%)	37,89,113	1.81	8 (21%)
19	CLA	AA	825	-	44,60,73	1.16	4 (9%)	50,97,113	1.56	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	AA	826	-	34,53,73	1.28	5 (14%)	37,89,113	1.71	7 (18%)
19	CLA	AA	827	-	57,73,73	1.05	5 (8%)	66,113,113	1.33	4 (6%)
19	CLA	AA	828	-	48,64,73	1.11	4 (8%)	55,102,113	1.59	8 (14%)
19	CLA	AA	829	-	57,73,73	1.02	4 (7%)	66,113,113	1.49	9 (13%)
19	CLA	AA	830	-	54,70,73	1.01	5 (9%)	62,109,113	1.48	9 (14%)
19	CLA	AA	831	-	57,73,73	1.05	4 (7%)	66,113,113	1.40	9 (13%)
19	CLA	AA	832	-	57,73,73	1.02	5 (8%)	66,113,113	1.47	10 (15%)
19	CLA	AA	833	-	42,58,73	1.20	6 (14%)	48,95,113	1.46	5 (10%)
19	CLA	AA	834	-	33,49,73	1.31	5 (15%)	37,84,113	1.73	8 (21%)
19	CLA	AA	835	-	57,73,73	1.07	4 (7%)	66,113,113	1.41	9 (13%)
19	CLA	AA	836	-	57,73,73	1.03	6 (10%)	66,113,113	1.42	7 (10%)
19	CLA	AA	837	-	34,53,73	1.31	5 (14%)	37,89,113	1.75	8 (21%)
19	CLA	AA	838	-	36,52,73	1.25	4 (11%)	39,87,113	1.83	8 (20%)
19	CLA	AA	839	-	44,60,73	1.16	4 (9%)	50,97,113	1.61	8 (16%)
19	CLA	AA	840	-	48,64,73	1.11	5 (10%)	55,102,113	1.47	6 (10%)
19	CLA	AA	841	-	38,54,73	1.21	4 (10%)	43,90,113	1.71	8 (18%)
19	CLA	AA	842	-	57,73,73	1.04	6 (10%)	66,113,113	1.53	11 (16%)
19	CLA	AA	843	-	57,73,73	1.07	5 (8%)	66,113,113	1.65	11 (16%)
21	PQN	AA	844	-	34,34,34	0.64	0	42,45,45	1.03	3 (7%)
19	CLA	AA	845	-	33,49,73	1.30	4 (12%)	37,84,113	1.82	7 (18%)
22	LHG	AA	846	-	48,48,48	0.79	2 (4%)	51,54,54	0.96	3 (5%)
22	LHG	AA	847	-	37,37,48	0.81	1 (2%)	40,43,54	1.00	3 (7%)
23	BCR	AA	848	-	40,40,41	1.09	2 (5%)	53,54,56	1.25	9 (16%)
23	BCR	AA	849	-	41,41,41	1.14	2 (4%)	56,56,56	1.20	7 (12%)
23	BCR	AA	850	-	41,41,41	1.05	2 (4%)	56,56,56	1.26	8 (14%)
23	BCR	AA	851	-	41,41,41	1.13	2 (4%)	56,56,56	1.24	5 (8%)
23	BCR	AA	852	-	41,41,41	1.09	1 (2%)	56,56,56	1.44	7 (12%)
19	CLA	AA	853	-	57,73,73	1.07	7 (12%)	66,113,113	1.38	10 (15%)
23	BCR	AA	854	-	41,41,41	1.13	2 (4%)	56,56,56	1.36	12 (21%)
23	BCR	AA	855	-	41,41,41	1.14	2 (4%)	56,56,56	1.29	8 (14%)
24	AJP	AA	856	-	40,40,95	4.24	24 (60%)	57,65,149	3.45	19 (33%)
19	CLA	B	801	-	57,73,73	1.00	4 (7%)	66,113,113	1.77	14 (21%)
19	CLA	B	802	-	57,73,73	1.06	6 (10%)	66,113,113	1.42	8 (12%)
19	CLA	B	803	-	57,73,73	1.04	5 (8%)	66,113,113	1.53	9 (13%)
19	CLA	B	804	-	54,70,73	1.07	5 (9%)	62,109,113	1.48	11 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	805	-	56,72,73	1.04	6 (10%)	64,111,113	1.57	11 (17%)
19	CLA	B	806	-	57,73,73	1.03	5 (8%)	66,113,113	1.55	11 (16%)
19	CLA	B	807	-	57,73,73	1.04	4 (7%)	66,113,113	1.52	8 (12%)
19	CLA	B	808	-	52,68,73	1.09	4 (7%)	60,107,113	1.37	7 (11%)
19	CLA	B	809	-	34,53,73	1.29	5 (14%)	37,89,113	1.81	9 (24%)
19	CLA	B	810	-	57,73,73	1.03	5 (8%)	66,113,113	1.49	9 (13%)
19	CLA	B	811	-	53,69,73	1.05	5 (9%)	61,108,113	1.39	6 (9%)
19	CLA	B	812	-	33,49,73	1.28	4 (12%)	37,84,113	1.91	10 (27%)
19	CLA	B	813	-	34,50,73	1.30	5 (14%)	38,85,113	1.69	9 (23%)
19	CLA	B	814	-	51,67,73	1.12	5 (9%)	58,105,113	1.60	11 (18%)
19	CLA	B	815	-	57,73,73	1.01	4 (7%)	66,113,113	1.58	11 (16%)
19	CLA	B	816	-	49,65,73	1.16	6 (12%)	56,103,113	1.54	9 (16%)
19	CLA	B	817	-	34,50,73	1.28	4 (11%)	38,85,113	1.84	9 (23%)
19	CLA	B	818	-	33,49,73	1.20	3 (9%)	37,84,113	1.67	6 (16%)
19	CLA	B	819	-	33,49,73	1.29	4 (12%)	37,84,113	1.78	8 (21%)
19	CLA	B	820	-	34,53,73	1.34	5 (14%)	37,89,113	2.09	11 (29%)
19	CLA	B	821	2	57,73,73	1.00	4 (7%)	66,113,113	1.50	8 (12%)
19	CLA	B	822	-	57,73,73	1.04	5 (8%)	66,113,113	1.45	7 (10%)
19	CLA	B	823	-	57,73,73	1.04	5 (8%)	66,113,113	1.44	6 (9%)
19	CLA	B	824	-	47,63,73	1.13	4 (8%)	54,101,113	1.49	8 (14%)
19	CLA	B	825	-	57,73,73	1.03	4 (7%)	66,113,113	1.47	8 (12%)
19	CLA	B	826	-	57,73,73	1.08	6 (10%)	66,113,113	1.57	12 (18%)
19	CLA	B	827	-	34,53,73	1.32	5 (14%)	37,89,113	1.67	6 (16%)
19	CLA	B	828	-	34,53,73	1.27	5 (14%)	37,89,113	1.71	7 (18%)
19	CLA	B	829	-	57,73,73	1.04	4 (7%)	66,113,113	1.41	8 (12%)
19	CLA	B	830	-	48,64,73	1.10	5 (10%)	55,102,113	1.60	11 (20%)
19	CLA	B	831	-	48,64,73	1.11	4 (8%)	55,102,113	1.51	9 (16%)
19	CLA	B	832	-	34,53,73	1.35	6 (17%)	37,89,113	1.60	5 (13%)
19	CLA	B	833	-	57,73,73	1.06	5 (8%)	66,113,113	1.60	13 (19%)
19	CLA	B	834	-	57,73,73	1.09	6 (10%)	66,113,113	1.76	16 (24%)
19	CLA	B	835	-	34,53,73	1.29	4 (11%)	37,89,113	1.76	8 (21%)
19	CLA	B	836	-	57,73,73	1.05	5 (8%)	66,113,113	1.43	9 (13%)
19	CLA	B	837	-	52,68,73	1.09	5 (9%)	60,107,113	1.46	7 (11%)
21	PQN	B	838	-	34,34,34	0.63	0	42,45,45	0.85	1 (2%)
23	BCR	B	839	-	41,41,41	1.14	2 (4%)	56,56,56	1.27	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCR	B	840	-	41,41,41	1.10	2 (4%)	56,56,56	1.20	6 (10%)
26	ECH	B	841	-	42,42,42	0.89	1 (2%)	55,58,58	2.49	22 (40%)
23	BCR	B	842	-	41,41,41	1.09	2 (4%)	56,56,56	1.34	6 (10%)
23	BCR	B	843	-	41,41,41	1.19	2 (4%)	56,56,56	1.18	6 (10%)
23	BCR	B	844	-	41,41,41	1.24	4 (9%)	56,56,56	1.22	7 (12%)
25	LMG	B	845	-	55,55,55	0.69	0	63,63,63	1.25	4 (6%)
19	CLA	B	846	-	31,47,73	1.29	4 (12%)	33,80,113	1.92	9 (27%)
23	BCR	B	848	-	41,41,41	1.17	2 (4%)	56,56,56	1.34	8 (14%)
24	AJP	B	849	-	49,49,95	3.88	23 (46%)	71,80,149	4.32	42 (59%)
24	AJP	B	850	-	49,49,95	3.89	25 (51%)	71,80,149	4.24	43 (60%)
25	LMG	B	851	-	55,55,55	0.67	0	63,63,63	1.27	7 (11%)
22	LHG	B	852	-	32,32,48	0.89	1 (3%)	35,38,54	1.01	3 (8%)
22	LHG	B	853	-	48,48,48	0.75	1 (2%)	51,54,54	0.97	4 (7%)
19	CLA	B	854	-	57,73,73	1.03	6 (10%)	66,113,113	1.47	5 (7%)
28	DGD	B	856	-	43,43,67	1.06	0	57,57,81	1.39	6 (10%)
24	AJP	B	857	-	49,49,95	3.87	25 (51%)	71,80,149	3.20	20 (28%)
19	CLA	B	858	-	57,73,73	1.06	5 (8%)	66,113,113	1.41	10 (15%)
19	CLA	B	859	-	52,68,73	1.10	6 (11%)	60,107,113	1.84	17 (28%)
19	CLA	B	860	-	57,73,73	1.07	5 (8%)	66,113,113	1.68	12 (18%)
27	SF4	B	861	-	0,12,12	0.00	-	-	-	-
19	CLA	B1	801	-	57,73,73	1.01	4 (7%)	66,113,113	1.63	11 (16%)
19	CLA	B1	802	-	57,73,73	1.04	5 (8%)	66,113,113	1.40	10 (15%)
19	CLA	B1	803	-	57,73,73	1.05	7 (12%)	66,113,113	1.49	9 (13%)
19	CLA	B1	804	-	54,70,73	1.07	5 (9%)	62,109,113	1.50	10 (16%)
19	CLA	B1	805	-	56,72,73	1.04	6 (10%)	64,111,113	1.57	11 (17%)
19	CLA	B1	806	-	57,73,73	1.02	5 (8%)	66,113,113	1.56	12 (18%)
19	CLA	B1	807	-	57,73,73	1.06	4 (7%)	66,113,113	1.61	11 (16%)
19	CLA	B1	808	-	52,68,73	1.08	4 (7%)	60,107,113	1.42	7 (11%)
19	CLA	B1	809	-	34,53,73	1.28	4 (11%)	37,89,113	1.78	9 (24%)
19	CLA	B1	810	-	57,73,73	1.03	4 (7%)	66,113,113	1.45	11 (16%)
19	CLA	B1	811	-	53,69,73	1.07	4 (7%)	61,108,113	1.36	6 (9%)
19	CLA	B1	812	-	33,49,73	1.28	4 (12%)	37,84,113	1.83	7 (18%)
19	CLA	B1	813	-	34,50,73	1.29	4 (11%)	38,85,113	1.69	9 (23%)
19	CLA	B1	814	-	51,67,73	1.11	4 (7%)	58,105,113	1.47	8 (13%)
19	CLA	B1	815	-	57,73,73	1.01	4 (7%)	66,113,113	1.63	11 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B1	816	-	49,65,73	1.14	5 (10%)	56,103,113	1.47	8 (14%)
19	CLA	B1	817	-	34,50,73	1.28	4 (11%)	38,85,113	1.76	7 (18%)
19	CLA	B1	818	-	33,49,73	1.28	4 (12%)	37,84,113	1.73	7 (18%)
19	CLA	B1	819	-	33,49,73	1.28	4 (12%)	37,84,113	1.78	9 (24%)
19	CLA	B1	820	-	34,53,73	1.30	4 (11%)	37,89,113	1.71	9 (24%)
19	CLA	B1	821	2	57,73,73	1.01	5 (8%)	66,113,113	1.47	10 (15%)
19	CLA	B1	822	-	57,73,73	1.03	5 (8%)	66,113,113	1.41	9 (13%)
19	CLA	B1	823	-	57,73,73	1.03	4 (7%)	66,113,113	1.45	7 (10%)
19	CLA	B1	824	-	47,63,73	1.18	6 (12%)	54,101,113	1.48	9 (16%)
19	CLA	B1	825	-	57,73,73	1.03	4 (7%)	66,113,113	1.49	8 (12%)
19	CLA	B1	826	-	57,73,73	1.08	6 (10%)	66,113,113	1.58	12 (18%)
19	CLA	B1	827	-	34,53,73	1.31	5 (14%)	37,89,113	1.65	6 (16%)
19	CLA	B1	828	-	57,73,73	1.04	4 (7%)	66,113,113	1.36	8 (12%)
19	CLA	B1	829	-	48,64,73	1.14	7 (14%)	55,102,113	1.59	10 (18%)
19	CLA	B1	830	-	48,64,73	1.11	4 (8%)	55,102,113	1.52	8 (14%)
19	CLA	B1	831	-	34,53,73	1.33	6 (17%)	37,89,113	1.61	5 (13%)
19	CLA	B1	832	-	57,73,73	1.02	4 (7%)	66,113,113	1.53	11 (16%)
19	CLA	B1	833	-	57,73,73	1.09	7 (12%)	66,113,113	1.79	16 (24%)
19	CLA	B1	834	-	34,53,73	1.27	4 (11%)	37,89,113	1.73	7 (18%)
19	CLA	B1	835	-	57,73,73	1.04	6 (10%)	66,113,113	1.36	7 (10%)
19	CLA	B1	836	-	52,68,73	1.09	4 (7%)	60,107,113	1.56	9 (15%)
21	PQN	B1	837	-	34,34,34	0.70	0	42,45,45	0.86	0
23	BCR	B1	838	-	41,41,41	1.13	2 (4%)	56,56,56	1.32	10 (17%)
23	BCR	B1	839	-	41,41,41	1.10	2 (4%)	56,56,56	1.16	3 (5%)
26	ECH	B1	840	-	42,42,42	0.81	1 (2%)	55,58,58	2.43	19 (34%)
23	BCR	B1	841	-	41,41,41	1.06	2 (4%)	56,56,56	1.35	6 (10%)
23	BCR	B1	842	-	41,41,41	1.18	2 (4%)	56,56,56	1.22	6 (10%)
23	BCR	B1	843	-	41,41,41	1.21	3 (7%)	56,56,56	1.19	6 (10%)
25	LMG	B1	844	-	55,55,55	0.68	0	63,63,63	1.27	3 (4%)
19	CLA	B1	845	-	31,47,73	1.29	4 (12%)	33,80,113	1.87	9 (27%)
25	LMG	B1	846	-	32,32,55	0.93	0	40,40,63	1.20	4 (10%)
22	LHG	B1	847	-	32,32,48	0.87	1 (3%)	35,38,54	1.03	3 (8%)
19	CLA	B1	848	-	57,73,73	1.06	6 (10%)	66,113,113	1.48	6 (9%)
19	CLA	B1	849	-	57,73,73	1.05	6 (10%)	66,113,113	1.35	7 (10%)
19	CLA	B1	850	-	52,68,73	1.10	5 (9%)	60,107,113	1.80	17 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	SF4	B1	851	-	0,12,12	0.00	-	-		
25	LMG	B1	852	-	30,30,55	0.99	0	38,38,63	1.22	4 (10%)
19	CLA	B2	801	-	57,73,73	1.01	4 (7%)	66,113,113	1.65	11 (16%)
19	CLA	B2	802	-	57,73,73	1.05	4 (7%)	66,113,113	1.42	9 (13%)
19	CLA	B2	803	-	57,73,73	1.04	6 (10%)	66,113,113	1.53	9 (13%)
19	CLA	B2	804	-	54,70,73	1.07	6 (11%)	62,109,113	1.52	10 (16%)
19	CLA	B2	805	-	56,72,73	1.04	5 (8%)	64,111,113	1.57	11 (17%)
19	CLA	B2	806	2	57,73,73	1.02	5 (8%)	66,113,113	1.53	11 (16%)
19	CLA	B2	807	-	57,73,73	1.06	4 (7%)	66,113,113	1.63	11 (16%)
19	CLA	B2	808	-	52,68,73	1.08	4 (7%)	60,107,113	1.44	7 (11%)
19	CLA	B2	809	-	34,53,73	1.28	4 (11%)	37,89,113	1.78	9 (24%)
19	CLA	B2	810	-	57,73,73	1.02	4 (7%)	66,113,113	1.45	10 (15%)
19	CLA	B2	811	-	53,69,73	1.06	4 (7%)	61,108,113	1.37	6 (9%)
19	CLA	B2	812	-	33,49,73	1.28	4 (12%)	37,84,113	1.84	8 (21%)
19	CLA	B2	813	-	34,50,73	1.28	4 (11%)	38,85,113	1.67	9 (23%)
19	CLA	B2	814	-	51,67,73	1.12	5 (9%)	58,105,113	1.47	7 (12%)
19	CLA	B2	815	-	57,73,73	1.03	4 (7%)	66,113,113	1.56	11 (16%)
19	CLA	B2	816	-	49,65,73	1.13	5 (10%)	56,103,113	1.50	7 (12%)
19	CLA	B2	817	-	34,50,73	1.28	4 (11%)	38,85,113	1.77	8 (21%)
19	CLA	B2	818	-	33,49,73	1.28	4 (12%)	37,84,113	1.73	8 (21%)
19	CLA	B2	819	-	33,49,73	1.29	5 (15%)	37,84,113	1.83	8 (21%)
19	CLA	B2	820	-	34,53,73	1.34	5 (14%)	37,89,113	1.99	12 (32%)
19	CLA	B2	821	-	57,73,73	1.00	4 (7%)	66,113,113	1.51	11 (16%)
19	CLA	B2	822	-	57,73,73	1.06	5 (8%)	66,113,113	1.45	8 (12%)
19	CLA	B2	823	-	57,73,73	1.03	4 (7%)	66,113,113	1.46	7 (10%)
19	CLA	B2	824	-	47,63,73	1.14	4 (8%)	54,101,113	1.54	8 (14%)
19	CLA	B2	825	-	57,73,73	1.03	4 (7%)	66,113,113	1.49	9 (13%)
19	CLA	B2	826	-	57,73,73	1.07	5 (8%)	66,113,113	1.58	11 (16%)
19	CLA	B2	827	-	34,53,73	1.33	6 (17%)	37,89,113	1.65	6 (16%)
19	CLA	B2	828	-	34,53,73	1.26	4 (11%)	37,89,113	1.71	7 (18%)
19	CLA	B2	829	-	57,73,73	1.05	4 (7%)	66,113,113	1.33	7 (10%)
19	CLA	B2	830	-	48,64,73	1.14	7 (14%)	55,102,113	1.60	10 (18%)
19	CLA	B2	831	-	48,64,73	1.10	4 (8%)	55,102,113	1.54	8 (14%)
19	CLA	B2	832	-	34,53,73	1.31	5 (14%)	37,89,113	1.59	5 (13%)
19	CLA	B2	833	-	57,73,73	1.02	4 (7%)	66,113,113	1.64	13 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B2	834	-	57,73,73	1.11	6 (10%)	66,113,113	1.74	15 (22%)
19	CLA	B2	835	-	34,53,73	1.29	4 (11%)	37,89,113	1.68	6 (16%)
19	CLA	B2	836	-	57,73,73	1.05	6 (10%)	66,113,113	1.36	6 (9%)
19	CLA	B2	837	-	52,68,73	1.09	4 (7%)	60,107,113	1.54	9 (15%)
21	PQN	B2	838	-	34,34,34	0.61	0	42,45,45	0.84	0
23	BCR	B2	839	-	41,41,41	1.13	2 (4%)	56,56,56	1.33	10 (17%)
23	BCR	B2	840	-	41,41,41	1.09	2 (4%)	56,56,56	1.20	5 (8%)
26	ECH	B2	841	-	42,42,42	0.79	1 (2%)	55,58,58	2.41	18 (32%)
23	BCR	B2	842	-	41,41,41	1.01	2 (4%)	56,56,56	1.35	7 (12%)
23	BCR	B2	843	-	41,41,41	1.16	2 (4%)	56,56,56	1.17	6 (10%)
23	BCR	B2	844	-	41,41,41	1.21	3 (7%)	56,56,56	1.19	6 (10%)
25	LMG	B2	845	-	55,55,55	0.68	0	63,63,63	1.26	4 (6%)
19	CLA	B2	846	-	31,47,73	1.29	4 (12%)	33,80,113	1.87	9 (27%)
25	LMG	B2	847	-	32,32,55	0.93	0	40,40,63	1.21	2 (5%)
22	LHG	B2	848	-	32,32,48	0.89	2 (6%)	35,38,54	0.98	2 (5%)
19	CLA	B2	849	-	57,73,73	1.05	5 (8%)	66,113,113	1.46	5 (7%)
19	CLA	B2	850	-	57,73,73	1.07	7 (12%)	66,113,113	1.40	7 (10%)
19	CLA	B2	851	-	52,68,73	1.09	5 (9%)	60,107,113	1.81	16 (26%)
19	CLA	B2	852	-	57,73,73	1.07	5 (8%)	66,113,113	1.66	12 (18%)
27	SF4	B2	853	-	0,12,12	0.00	-	-	-	-
25	LMG	B2	854	-	30,30,55	0.99	0	38,38,63	1.22	4 (10%)
19	CLA	BB	801	-	57,73,73	1.00	4 (7%)	66,113,113	1.75	11 (16%)
19	CLA	BB	802	-	57,73,73	1.07	6 (10%)	66,113,113	1.40	9 (13%)
19	CLA	BB	803	-	57,73,73	1.04	5 (8%)	66,113,113	1.50	9 (13%)
19	CLA	BB	804	-	54,70,73	1.07	6 (11%)	62,109,113	1.49	11 (17%)
19	CLA	BB	805	-	56,72,73	1.04	6 (10%)	64,111,113	1.56	11 (17%)
19	CLA	BB	806	-	57,73,73	1.04	5 (8%)	66,113,113	1.52	12 (18%)
19	CLA	BB	807	-	57,73,73	1.04	4 (7%)	66,113,113	1.53	8 (12%)
19	CLA	BB	808	-	52,68,73	1.11	5 (9%)	60,107,113	1.45	8 (13%)
19	CLA	BB	809	-	34,53,73	1.29	5 (14%)	37,89,113	1.82	9 (24%)
19	CLA	BB	810	-	57,73,73	1.02	4 (7%)	66,113,113	1.44	10 (15%)
19	CLA	BB	811	-	53,69,73	1.06	5 (9%)	61,108,113	1.41	7 (11%)
19	CLA	BB	812	-	33,49,73	1.30	4 (12%)	37,84,113	1.82	8 (21%)
19	CLA	BB	813	-	34,50,73	1.28	4 (11%)	38,85,113	1.75	9 (23%)
19	CLA	BB	814	-	51,67,73	1.12	7 (13%)	58,105,113	1.57	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	BB	815	-	57,73,73	1.02	4 (7%)	66,113,113	1.56	9 (13%)
19	CLA	BB	816	-	49,65,73	1.15	6 (12%)	56,103,113	1.54	9 (16%)
19	CLA	BB	817	-	34,50,73	1.28	4 (11%)	38,85,113	1.79	8 (21%)
19	CLA	BB	818	-	33,49,73	1.34	4 (12%)	37,84,113	1.64	6 (16%)
19	CLA	BB	819	-	33,49,73	1.28	4 (12%)	37,84,113	1.80	10 (27%)
19	CLA	BB	820	-	34,53,73	1.36	5 (14%)	37,89,113	2.14	13 (35%)
19	CLA	BB	821	-	57,73,73	1.01	4 (7%)	66,113,113	1.39	8 (12%)
19	CLA	BB	822	-	57,73,73	1.01	6 (10%)	66,113,113	1.46	6 (9%)
19	CLA	BB	823	-	57,73,73	1.04	5 (8%)	66,113,113	1.44	7 (10%)
19	CLA	BB	824	-	47,63,73	1.15	5 (10%)	54,101,113	1.51	8 (14%)
19	CLA	BB	825	-	57,73,73	1.03	4 (7%)	66,113,113	1.47	8 (12%)
19	CLA	BB	826	-	57,73,73	1.12	6 (10%)	66,113,113	1.59	12 (18%)
19	CLA	BB	827	-	34,53,73	1.32	6 (17%)	37,89,113	1.66	6 (16%)
19	CLA	BB	828	-	34,53,73	1.27	5 (14%)	37,89,113	1.76	7 (18%)
19	CLA	BB	829	-	48,64,73	1.17	6 (12%)	55,102,113	1.54	10 (18%)
19	CLA	BB	830	-	48,64,73	1.11	4 (8%)	55,102,113	1.50	9 (16%)
19	CLA	BB	831	-	34,53,73	1.35	6 (17%)	37,89,113	1.66	6 (16%)
19	CLA	BB	832	-	57,73,73	1.08	6 (10%)	66,113,113	1.58	11 (16%)
19	CLA	BB	833	-	57,73,73	1.08	6 (10%)	66,113,113	1.76	16 (24%)
19	CLA	BB	834	-	34,53,73	1.28	5 (14%)	37,89,113	1.76	6 (16%)
19	CLA	BB	835	-	57,73,73	1.06	6 (10%)	66,113,113	1.39	9 (13%)
19	CLA	BB	836	-	52,68,73	1.12	5 (9%)	60,107,113	1.87	13 (21%)
21	PQN	BB	837	-	34,34,34	0.65	0	42,45,45	0.83	0
23	BCR	BB	838	-	41,41,41	1.16	2 (4%)	56,56,56	1.26	7 (12%)
23	BCR	BB	839	-	41,41,41	1.10	2 (4%)	56,56,56	1.20	6 (10%)
26	ECH	BB	840	-	42,42,42	0.88	0	55,58,58	2.44	18 (32%)
23	BCR	BB	841	-	41,41,41	1.09	2 (4%)	56,56,56	1.35	6 (10%)
23	BCR	BB	842	-	41,41,41	1.19	2 (4%)	56,56,56	1.19	5 (8%)
23	BCR	BB	843	-	41,41,41	1.21	4 (9%)	56,56,56	1.19	6 (10%)
25	LMG	BB	844	-	55,55,55	0.69	1 (1%)	63,63,63	1.26	4 (6%)
19	CLA	BB	845	-	31,47,73	1.29	4 (12%)	33,80,113	1.93	9 (27%)
23	BCR	BB	847	-	41,41,41	1.17	2 (4%)	56,56,56	1.34	8 (14%)
24	AJP	BB	848	-	49,49,95	3.87	24 (48%)	71,80,149	4.25	40 (56%)
24	AJP	BB	849	-	49,49,95	3.92	25 (51%)	71,80,149	4.23	44 (61%)
22	LHG	BB	850	-	32,32,48	0.89	1 (3%)	35,38,54	1.02	3 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	LHG	BB	851	-	48,48,48	0.76	2 (4%)	51,54,54	0.97	4 (7%)
19	CLA	BB	852	-	57,73,73	1.04	5 (8%)	66,113,113	1.53	7 (10%)
28	DGD	BB	854	-	43,43,67	1.05	0	57,57,81	1.40	7 (12%)
19	CLA	BB	855	-	57,73,73	1.05	7 (12%)	66,113,113	1.45	7 (10%)
19	CLA	BB	856	-	52,68,73	1.10	6 (11%)	60,107,113	1.83	17 (28%)
27	SF4	BB	857	-	0,12,12	0.00	-	-	-	-
27	SF4	C	101	-	0,12,12	0.00	-	-	-	-
27	SF4	C	102	3	0,12,12	0.00	-	-	-	-
27	SF4	C1	101	-	0,12,12	0.00	-	-	-	-
27	SF4	C1	102	-	0,12,12	0.00	-	-	-	-
27	SF4	C2	101	-	0,12,12	0.00	-	-	-	-
27	SF4	C2	102	-	0,12,12	0.00	-	-	-	-
27	SF4	CC	101	-	0,12,12	0.00	-	-	-	-
27	SF4	CC	102	-	0,12,12	0.00	-	-	-	-
19	CLA	F	301	-	52,68,73	1.06	5 (9%)	60,107,113	1.66	11 (18%)
19	CLA	F	302	-	34,50,73	1.28	4 (11%)	38,85,113	1.82	9 (23%)
23	BCR	F	303	-	41,41,41	1.13	2 (4%)	56,56,56	1.31	9 (16%)
23	BCR	F	304	-	41,41,41	1.21	2 (4%)	56,56,56	1.29	9 (16%)
23	BCR	F	305	-	41,41,41	1.15	3 (7%)	56,56,56	1.49	10 (17%)
19	CLA	F1	301	-	52,68,73	1.07	5 (9%)	60,107,113	1.65	11 (18%)
19	CLA	F1	302	-	34,50,73	1.28	5 (14%)	38,85,113	1.85	10 (26%)
23	BCR	F1	303	-	41,41,41	1.09	2 (4%)	56,56,56	1.27	7 (12%)
23	BCR	F1	304	-	41,41,41	1.21	2 (4%)	56,56,56	1.28	9 (16%)
19	CLA	F1	305	-	34,53,73	1.26	4 (11%)	37,89,113	1.71	7 (18%)
23	BCR	F1	306	-	41,41,41	1.12	2 (4%)	56,56,56	1.48	8 (14%)
19	CLA	F2	301	-	52,68,73	1.06	5 (9%)	60,107,113	1.60	11 (18%)
19	CLA	F2	302	-	34,50,73	1.28	5 (14%)	38,85,113	1.85	9 (23%)
23	BCR	F2	303	-	41,41,41	1.09	2 (4%)	56,56,56	1.29	8 (14%)
23	BCR	F2	304	-	41,41,41	1.20	2 (4%)	56,56,56	1.25	9 (16%)
23	BCR	F2	305	-	41,41,41	1.12	2 (4%)	56,56,56	1.48	9 (16%)
19	CLA	FF	301	-	52,68,73	1.08	4 (7%)	60,107,113	1.51	12 (20%)
19	CLA	FF	302	-	34,50,73	1.28	4 (11%)	38,85,113	1.83	9 (23%)
23	BCR	FF	303	-	41,41,41	1.12	2 (4%)	56,56,56	1.33	9 (16%)
23	BCR	FF	304	-	41,41,41	1.22	2 (4%)	56,56,56	1.29	9 (16%)
19	CLA	FF	305	-	57,73,73	1.04	4 (7%)	66,113,113	1.39	8 (12%)
23	BCR	FF	306	-	41,41,41	1.15	3 (7%)	56,56,56	1.48	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCR	I	101	-	41,41,41	1.18	2 (4%)	56,56,56	1.21	6 (10%)
23	BCR	I	102	-	41,41,41	1.15	2 (4%)	56,56,56	1.19	7 (12%)
23	BCR	I1	101	-	41,41,41	1.23	2 (4%)	56,56,56	1.27	8 (14%)
25	LMG	I1	102	-	35,35,55	1.04	1 (2%)	43,43,63	1.26	3 (6%)
23	BCR	I2	101	-	41,41,41	1.22	2 (4%)	56,56,56	1.27	9 (16%)
23	BCR	I2	102	-	41,41,41	1.16	2 (4%)	56,56,56	1.23	6 (10%)
23	BCR	I2	103	-	41,41,41	1.13	2 (4%)	56,56,56	1.36	9 (16%)
24	AJP	I2	104	-	36,36,95	4.36	22 (61%)	54,60,149	4.41	31 (57%)
25	LMG	I2	105	-	35,35,55	0.92	1 (2%)	43,43,63	1.21	4 (9%)
23	BCR	II	101	-	41,41,41	1.19	2 (4%)	56,56,56	1.22	8 (14%)
23	BCR	II	102	-	41,41,41	1.15	3 (7%)	56,56,56	1.19	5 (8%)
23	BCR	II	104	-	41,41,41	1.15	2 (4%)	56,56,56	1.32	8 (14%)
25	LMG	II	105	-	42,42,55	0.82	1 (2%)	50,50,63	1.23	5 (10%)
19	CLA	J	101	8	33,49,73	1.30	4 (12%)	37,84,113	1.76	8 (21%)
23	BCR	J	102	-	41,41,41	1.24	2 (4%)	56,56,56	1.38	9 (16%)
19	CLA	J	103	-	33,49,73	1.31	5 (15%)	37,84,113	1.70	7 (18%)
23	BCR	J	104	-	41,41,41	1.12	2 (4%)	56,56,56	1.36	7 (12%)
19	CLA	J1	101	-	33,49,73	1.30	4 (12%)	37,84,113	1.73	8 (21%)
23	BCR	J1	102	-	41,41,41	1.20	2 (4%)	56,56,56	1.36	9 (16%)
19	CLA	J1	103	-	33,49,73	1.30	4 (12%)	37,84,113	1.73	7 (18%)
23	BCR	J1	104	-	41,41,41	1.13	2 (4%)	56,56,56	1.33	6 (10%)
19	CLA	J2	101	8	33,49,73	1.31	4 (12%)	37,84,113	1.71	8 (21%)
23	BCR	J2	102	-	41,41,41	1.19	2 (4%)	56,56,56	1.35	8 (14%)
19	CLA	J2	103	-	33,49,73	1.30	4 (12%)	37,84,113	1.70	7 (18%)
23	BCR	J2	104	-	41,41,41	1.15	2 (4%)	56,56,56	1.31	9 (16%)
19	CLA	JJ	101	8	33,49,73	1.30	4 (12%)	37,84,113	1.76	8 (21%)
23	BCR	JJ	102	-	41,41,41	1.24	2 (4%)	56,56,56	1.37	10 (17%)
19	CLA	JJ	103	-	33,49,73	1.31	4 (12%)	37,84,113	1.73	7 (18%)
23	BCR	JJ	104	-	41,41,41	1.17	3 (7%)	56,56,56	1.24	7 (12%)
19	CLA	K	101	-	34,53,73	1.27	4 (11%)	37,89,113	1.89	9 (24%)
19	CLA	K	102	-	38,54,73	1.21	4 (10%)	43,90,113	1.67	8 (18%)
23	BCR	K	103	-	41,41,41	1.12	3 (7%)	56,56,56	1.24	7 (12%)
24	AJP	K	104	-	47,47,95	3.94	24 (51%)	68,77,149	4.30	38 (55%)
19	CLA	K1	102	-	34,53,73	1.28	4 (11%)	37,89,113	1.89	9 (24%)
19	CLA	K1	103	-	38,54,73	1.23	4 (10%)	43,90,113	1.68	7 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCR	K1	104	-	41,41,41	1.15	3 (7%)	56,56,56	1.18	6 (10%)
19	CLA	K1	105	9	31,48,73	1.35	4 (12%)	35,82,113	1.92	11 (31%)
23	BCR	K1	106	-	41,41,41	1.14	2 (4%)	56,56,56	1.35	10 (17%)
19	CLA	K2	102	-	34,53,73	1.28	4 (11%)	37,89,113	1.80	9 (24%)
23	BCR	K2	103	-	41,41,41	1.15	3 (7%)	56,56,56	1.18	6 (10%)
19	CLA	K2	104	-	30,49,73	1.31	4 (13%)	31,83,113	1.93	9 (29%)
23	BCR	K2	105	-	41,41,41	1.13	2 (4%)	56,56,56	1.32	9 (16%)
19	CLA	KK	101	-	34,53,73	1.27	4 (11%)	37,89,113	1.89	9 (24%)
19	CLA	KK	102	-	38,54,73	1.22	4 (10%)	43,90,113	1.68	8 (18%)
23	BCR	KK	103	-	41,41,41	1.12	2 (4%)	56,56,56	1.34	9 (16%)
24	AJP	KK	104	-	47,47,95	3.93	24 (51%)	68,77,149	4.33	38 (55%)
19	CLA	L	202	18	53,69,73	1.07	5 (9%)	61,108,113	1.71	10 (16%)
19	CLA	L	203	-	57,73,73	1.07	6 (10%)	66,113,113	1.49	10 (15%)
19	CLA	L	204	-	57,73,73	1.01	4 (7%)	66,113,113	1.62	11 (16%)
23	BCR	L	205	-	41,41,41	1.14	2 (4%)	56,56,56	1.32	9 (16%)
23	BCR	L	206	-	41,41,41	1.17	2 (4%)	56,56,56	1.25	9 (16%)
22	LHG	L	207	-	33,33,48	0.94	3 (9%)	36,39,54	1.05	4 (11%)
24	AJP	L	208	-	36,36,95	4.44	24 (66%)	54,60,149	4.64	33 (61%)
24	AJP	L	209	-	36,36,95	4.47	24 (66%)	54,60,149	4.56	31 (57%)
23	BCR	L1	201	-	41,41,41	1.16	2 (4%)	56,56,56	1.23	6 (10%)
24	AJP	L1	203	-	49,49,95	3.87	24 (48%)	71,80,149	3.74	35 (49%)
24	AJP	L1	204	-	49,49,95	3.84	23 (46%)	71,80,149	4.02	45 (63%)
19	CLA	L1	205	10	53,69,73	1.06	4 (7%)	61,108,113	1.57	12 (19%)
19	CLA	L1	206	-	57,73,73	1.05	6 (10%)	66,113,113	1.52	10 (15%)
19	CLA	L1	207	-	57,73,73	0.98	4 (7%)	66,113,113	1.47	7 (10%)
23	BCR	L1	208	-	41,41,41	1.12	2 (4%)	56,56,56	1.35	10 (17%)
23	BCR	L1	209	-	41,41,41	1.14	2 (4%)	56,56,56	1.26	9 (16%)
25	LMG	L1	210	-	55,55,55	0.68	0	63,63,63	1.27	6 (9%)
22	LHG	L1	211	-	32,32,48	0.95	3 (9%)	35,38,54	1.02	3 (8%)
24	AJP	L2	202	-	49,49,95	3.88	23 (46%)	71,80,149	4.36	44 (61%)
24	AJP	L2	203	-	49,49,95	3.84	22 (44%)	71,80,149	4.02	44 (61%)
19	CLA	L2	204	16	53,69,73	1.06	4 (7%)	61,108,113	1.54	11 (18%)
19	CLA	L2	205	-	51,67,73	1.09	6 (11%)	58,105,113	1.67	9 (15%)
19	CLA	L2	206	-	57,73,73	0.98	4 (7%)	66,113,113	1.47	8 (12%)
23	BCR	L2	207	-	41,41,41	1.15	2 (4%)	56,56,56	1.27	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	LHG	L2	208	-	34,34,48	0.86	1 (2%)	37,40,54	1.05	3 (8%)
19	CLA	LL	201	18	53,69,73	1.07	4 (7%)	61,108,113	1.75	10 (16%)
19	CLA	LL	202	-	57,73,73	1.07	7 (12%)	66,113,113	1.53	10 (15%)
19	CLA	LL	203	-	34,50,73	1.32	4 (11%)	38,85,113	1.98	8 (21%)
23	BCR	LL	204	-	41,41,41	1.14	2 (4%)	56,56,56	1.19	6 (10%)
22	LHG	LL	205	-	33,33,48	0.94	3 (9%)	36,39,54	1.04	4 (11%)
23	BCR	M	101	-	41,41,41	1.21	3 (7%)	56,56,56	1.33	10 (17%)
25	LMG	M	102	-	46,46,55	0.82	0	54,54,63	1.27	7 (12%)
23	BCR	M1	101	-	41,41,41	1.13	3 (7%)	56,56,56	1.24	7 (12%)
24	AJP	M2	101	-	36,36,95	4.46	23 (63%)	54,60,149	4.47	30 (55%)
23	BCR	M2	102	-	41,41,41	1.12	3 (7%)	56,56,56	1.24	9 (16%)
23	BCR	MM	101	-	41,41,41	1.20	3 (7%)	56,56,56	1.36	10 (17%)
19	CLA	X	101	-	34,53,73	1.27	4 (11%)	37,89,113	1.77	7 (18%)
22	LHG	X	102	-	39,39,48	0.80	2 (5%)	42,45,54	0.94	2 (4%)
19	CLA	X1	101	-	34,53,73	1.26	4 (11%)	37,89,113	1.77	7 (18%)
22	LHG	X1	102	-	39,39,48	0.81	2 (5%)	42,45,54	0.93	2 (4%)
22	LHG	X1	103	-	48,48,48	0.76	1 (2%)	51,54,54	0.95	3 (5%)
19	CLA	X2	101	-	34,53,73	1.26	4 (11%)	37,89,113	1.74	7 (18%)
22	LHG	X2	102	-	39,39,48	0.81	2 (5%)	42,45,54	0.93	2 (4%)
22	LHG	X2	103	-	48,48,48	0.76	1 (2%)	51,54,54	0.95	4 (7%)
19	CLA	XX	101	-	34,53,73	1.27	4 (11%)	37,89,113	1.77	7 (18%)
22	LHG	XX	102	-	39,39,48	0.80	2 (5%)	42,45,54	0.93	2 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	801	-	3/3/25/25	11/37/135/135	-
24	AJP	A	802	-	3/3/14/38	-	0/6/6/11
20	CL0	A	803	-	4/4/25/25	18/37/135/135	-
19	CLA	A	804	-	3/3/25/25	17/37/135/135	-
19	CLA	A	805	-	3/3/24/25	8/31/129/135	-
19	CLA	A	806	-	3/3/23/25	8/27/125/135	-
19	CLA	A	807	-	3/3/25/25	17/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	808	-	3/3/25/25	13/37/135/135	-
19	CLA	A	809	-	3/3/22/25	2/19/117/135	-
19	CLA	A	810	1	3/3/25/25	11/37/135/135	-
19	CLA	A	811	1	3/3/22/25	6/21/119/135	-
19	CLA	A	812	-	3/3/20/25	7/15/113/135	-
19	CLA	A	813	-	3/3/25/25	9/37/135/135	-
19	CLA	A	814	-	3/3/19/25	3/10/108/135	-
19	CLA	A	815	-	3/3/23/25	9/25/123/135	-
19	CLA	A	816	-	3/3/22/25	7/19/117/135	-
19	CLA	A	817	-	3/3/19/25	3/11/110/135	-
19	CLA	A	818	-	3/3/20/25	1/11/111/135	-
19	CLA	A	819	-	3/3/24/25	11/31/129/135	-
19	CLA	A	820	-	2/2/23/25	11/29/127/135	-
19	CLA	A	821	-	3/3/25/25	13/37/135/135	-
19	CLA	A	822	-	3/3/22/25	7/21/119/135	-
19	CLA	A	823	-	3/3/24/25	14/31/129/135	-
19	CLA	A	824	-	3/3/20/25	9/11/111/135	-
19	CLA	A	825	-	3/3/22/25	3/22/120/135	-
19	CLA	A	826	-	3/3/20/25	7/11/111/135	-
19	CLA	A	827	-	3/3/25/25	16/37/135/135	-
19	CLA	A	828	-	3/3/23/25	11/27/125/135	-
19	CLA	A	829	-	3/3/25/25	14/37/135/135	-
19	CLA	A	830	-	3/3/24/25	15/34/132/135	-
19	CLA	A	831	-	3/3/25/25	12/37/135/135	-
19	CLA	A	832	-	3/3/25/25	9/37/135/135	-
19	CLA	A	833	-	3/3/22/25	5/19/117/135	-
19	CLA	A	834	-	3/3/19/25	4/8/106/135	-
19	CLA	A	835	-	3/3/25/25	8/37/135/135	-
19	CLA	A	836	-	3/3/25/25	13/37/135/135	-
19	CLA	A	837	-	3/3/20/25	2/11/111/135	-
19	CLA	A	838	-	3/3/19/25	5/11/110/135	-
19	CLA	A	839	-	3/3/22/25	8/22/120/135	-
19	CLA	A	840	-	3/3/23/25	5/27/125/135	-
19	CLA	A	841	-	3/3/20/25	4/15/113/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	842	-	3/3/25/25	11/37/135/135	-
21	PQN	A	843	-	-	8/23/43/43	0/2/2/2
19	CLA	A	844	-	3/3/19/25	4/8/106/135	-
22	LHG	A	845	-	-	19/53/53/53	-
22	LHG	A	846	-	-	12/42/42/53	-
23	BCR	A	847	-	-	14/27/61/63	0/2/2/2
23	BCR	A	848	-	-	19/29/63/63	0/2/2/2
23	BCR	A	849	-	-	18/29/63/63	0/2/2/2
23	BCR	A	850	-	-	15/29/63/63	0/2/2/2
23	BCR	A	851	-	-	19/29/63/63	0/2/2/2
19	CLA	A	852	-	3/3/25/25	16/37/135/135	-
23	BCR	A	853	-	-	18/29/63/63	0/2/2/2
23	BCR	A	854	-	-	18/29/63/63	0/2/2/2
24	AJP	A	855	-	-	2/4/99/220	1/6/6/11
19	CLA	A1	801	-	3/3/25/25	13/37/135/135	-
20	CL0	A1	802	-	4/4/25/25	13/37/135/135	-
19	CLA	A1	803	-	3/3/25/25	17/37/135/135	-
19	CLA	A1	804	-	3/3/24/25	9/31/129/135	-
19	CLA	A1	805	-	2/2/23/25	6/27/125/135	-
19	CLA	A1	806	-	3/3/25/25	16/37/135/135	-
19	CLA	A1	807	-	3/3/25/25	14/37/135/135	-
19	CLA	A1	808	-	3/3/22/25	1/19/117/135	-
19	CLA	A1	809	-	3/3/25/25	11/37/135/135	-
19	CLA	A1	810	-	3/3/22/25	7/21/119/135	-
19	CLA	A1	811	-	3/3/20/25	5/15/113/135	-
19	CLA	A1	812	-	3/3/25/25	9/37/135/135	-
19	CLA	A1	813	-	3/3/19/25	4/10/108/135	-
19	CLA	A1	814	-	3/3/23/25	9/25/123/135	-
19	CLA	A1	815	-	3/3/22/25	9/19/117/135	-
19	CLA	A1	816	-	3/3/19/25	2/11/110/135	-
19	CLA	A1	817	-	3/3/20/25	1/11/111/135	-
19	CLA	A1	818	-	3/3/24/25	13/31/129/135	-
19	CLA	A1	819	-	2/2/23/25	9/29/127/135	-
19	CLA	A1	820	-	3/3/25/25	18/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A1	821	-	3/3/22/25	4/21/119/135	-
19	CLA	A1	822	-	3/3/24/25	15/31/129/135	-
19	CLA	A1	823	-	3/3/20/25	6/11/111/135	-
19	CLA	A1	824	-	3/3/19/25	2/10/108/135	-
19	CLA	A1	825	-	3/3/20/25	7/11/111/135	-
19	CLA	A1	826	-	3/3/25/25	14/37/135/135	-
19	CLA	A1	827	-	3/3/23/25	11/27/125/135	-
19	CLA	A1	828	-	3/3/25/25	20/37/135/135	-
19	CLA	A1	829	-	3/3/24/25	16/34/132/135	-
19	CLA	A1	830	-	3/3/25/25	14/37/135/135	-
19	CLA	A1	831	-	3/3/25/25	8/37/135/135	-
19	CLA	A1	832	-	3/3/22/25	9/19/117/135	-
19	CLA	A1	833	-	3/3/19/25	4/8/106/135	-
19	CLA	A1	834	-	3/3/25/25	7/37/135/135	-
19	CLA	A1	835	-	3/3/25/25	11/37/135/135	-
19	CLA	A1	836	-	3/3/20/25	4/11/111/135	-
19	CLA	A1	837	1	3/3/19/25	4/11/110/135	-
19	CLA	A1	838	-	3/3/22/25	8/22/120/135	-
19	CLA	A1	839	-	3/3/23/25	7/27/125/135	-
19	CLA	A1	840	-	3/3/20/25	6/15/113/135	-
19	CLA	A1	841	-	3/3/25/25	9/37/135/135	-
19	CLA	A1	842	-	3/3/25/25	15/37/135/135	-
21	PQN	A1	843	-	-	8/23/43/43	0/2/2/2
19	CLA	A1	844	-	3/3/19/25	3/8/106/135	-
22	LHG	A1	845	-	-	20/53/53/53	-
22	LHG	A1	846	-	-	12/42/42/53	-
23	BCR	A1	847	-	-	12/27/61/63	0/2/2/2
23	BCR	A1	848	-	-	14/29/63/63	0/2/2/2
23	BCR	A1	849	-	-	14/29/63/63	0/2/2/2
23	BCR	A1	850	-	-	14/29/63/63	0/2/2/2
23	BCR	A1	851	-	-	19/29/63/63	0/2/2/2
19	CLA	A1	852	-	3/3/25/25	18/37/135/135	-
23	BCR	A1	853	-	-	16/29/63/63	0/2/2/2
24	AJP	A1	854	-	-	2/6/121/220	0/7/7/11

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	AJP	A1	855	-	-	-	0/6/6/11
19	CLA	A2	801	-	3/3/25/25	13/37/135/135	-
19	CLA	A2	802	-	3/3/20/25	9/15/113/135	-
20	CL0	A2	803	-	4/4/25/25	16/37/135/135	-
19	CLA	A2	804	-	3/3/25/25	19/37/135/135	-
19	CLA	A2	805	-	3/3/24/25	8/31/129/135	-
19	CLA	A2	806	-	3/3/23/25	9/27/125/135	-
19	CLA	A2	807	-	3/3/25/25	16/37/135/135	-
19	CLA	A2	808	-	3/3/25/25	15/37/135/135	-
19	CLA	A2	809	-	3/3/22/25	2/19/117/135	-
19	CLA	A2	810	1	3/3/25/25	9/37/135/135	-
19	CLA	A2	811	-	3/3/22/25	6/21/119/135	-
19	CLA	A2	812	-	3/3/20/25	5/15/113/135	-
19	CLA	A2	813	-	3/3/25/25	11/37/135/135	-
19	CLA	A2	814	-	3/3/19/25	4/10/108/135	-
19	CLA	A2	815	-	3/3/23/25	9/25/123/135	-
19	CLA	A2	816	-	3/3/22/25	6/19/117/135	-
19	CLA	A2	817	-	3/3/19/25	1/11/110/135	-
19	CLA	A2	818	-	3/3/20/25	1/11/111/135	-
19	CLA	A2	819	-	3/3/24/25	9/31/129/135	-
19	CLA	A2	820	-	3/3/23/25	11/29/127/135	-
19	CLA	A2	821	-	3/3/25/25	13/37/135/135	-
19	CLA	A2	822	-	3/3/22/25	5/21/119/135	-
19	CLA	A2	823	-	3/3/24/25	12/31/129/135	-
19	CLA	A2	824	-	3/3/20/25	4/11/111/135	-
19	CLA	A2	825	-	3/3/19/25	3/10/108/135	-
19	CLA	A2	826	-	3/3/20/25	7/11/111/135	-
19	CLA	A2	827	-	3/3/25/25	14/37/135/135	-
19	CLA	A2	828	-	3/3/23/25	11/27/125/135	-
19	CLA	A2	829	-	3/3/25/25	17/37/135/135	-
19	CLA	A2	830	-	3/3/24/25	18/34/132/135	-
19	CLA	A2	831	-	3/3/25/25	13/37/135/135	-
19	CLA	A2	832	-	3/3/25/25	6/37/135/135	-
19	CLA	A2	833	-	3/3/22/25	5/19/117/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A2	834	-	3/3/19/25	4/8/106/135	-
19	CLA	A2	835	-	3/3/25/25	7/37/135/135	-
19	CLA	A2	836	-	2/2/25/25	14/37/135/135	-
19	CLA	A2	837	-	3/3/20/25	4/11/111/135	-
19	CLA	A2	838	-	3/3/19/25	4/11/110/135	-
19	CLA	A2	839	-	3/3/22/25	8/22/120/135	-
19	CLA	A2	840	-	3/3/23/25	4/27/125/135	-
19	CLA	A2	841	-	3/3/20/25	6/15/113/135	-
19	CLA	A2	842	-	3/3/25/25	10/37/135/135	-
21	PQN	A2	843	-	-	8/23/43/43	0/2/2/2
19	CLA	A2	844	-	3/3/19/25	3/8/106/135	-
22	LHG	A2	845	-	-	16/53/53/53	-
22	LHG	A2	846	-	-	12/42/42/53	-
23	BCR	A2	847	-	-	12/27/61/63	0/2/2/2
23	BCR	A2	848	-	-	15/29/63/63	0/2/2/2
23	BCR	A2	849	-	-	13/29/63/63	0/2/2/2
23	BCR	A2	850	-	-	13/29/63/63	0/2/2/2
23	BCR	A2	851	-	-	17/29/63/63	0/2/2/2
19	CLA	A2	852	-	3/3/25/25	13/37/135/135	-
23	BCR	A2	853	-	-	17/29/63/63	0/2/2/2
24	AJP	A2	854	-	-	-	0/6/6/11
19	CLA	AA	801	-	3/3/25/25	13/37/135/135	-
24	AJP	AA	802	-	3/3/14/38	-	0/6/6/11
20	CL0	AA	803	-	4/4/25/25	15/37/135/135	-
19	CLA	AA	804	-	3/3/25/25	16/37/135/135	-
19	CLA	AA	805	-	3/3/24/25	8/31/129/135	-
19	CLA	AA	806	-	3/3/23/25	8/27/125/135	-
19	CLA	AA	807	-	3/3/25/25	16/37/135/135	-
19	CLA	AA	808	-	3/3/25/25	14/37/135/135	-
19	CLA	AA	809	-	3/3/22/25	2/19/117/135	-
19	CLA	AA	810	-	3/3/25/25	10/37/135/135	-
19	CLA	AA	811	1	3/3/22/25	6/21/119/135	-
19	CLA	AA	812	-	3/3/20/25	7/15/113/135	-
19	CLA	AA	813	-	3/3/25/25	9/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	AA	814	-	3/3/19/25	3/10/108/135	-
19	CLA	AA	815	-	3/3/23/25	9/25/123/135	-
19	CLA	AA	816	-	3/3/22/25	9/19/117/135	-
19	CLA	AA	817	-	3/3/19/25	2/11/110/135	-
19	CLA	AA	818	-	3/3/20/25	1/11/111/135	-
19	CLA	AA	819	-	3/3/24/25	13/31/129/135	-
19	CLA	AA	820	-	3/3/23/25	11/29/127/135	-
19	CLA	AA	821	-	3/3/25/25	15/37/135/135	-
19	CLA	AA	822	-	2/2/22/25	8/21/119/135	-
19	CLA	AA	823	-	3/3/24/25	13/31/129/135	-
19	CLA	AA	824	-	3/3/20/25	9/11/111/135	-
19	CLA	AA	825	-	3/3/22/25	2/22/120/135	-
19	CLA	AA	826	-	3/3/20/25	7/11/111/135	-
19	CLA	AA	827	-	3/3/25/25	16/37/135/135	-
19	CLA	AA	828	-	3/3/23/25	11/27/125/135	-
19	CLA	AA	829	-	3/3/25/25	14/37/135/135	-
19	CLA	AA	830	-	3/3/24/25	14/34/132/135	-
19	CLA	AA	831	-	3/3/25/25	13/37/135/135	-
19	CLA	AA	832	-	3/3/25/25	6/37/135/135	-
19	CLA	AA	833	-	3/3/22/25	4/19/117/135	-
19	CLA	AA	834	-	3/3/19/25	4/8/106/135	-
19	CLA	AA	835	-	3/3/25/25	8/37/135/135	-
19	CLA	AA	836	-	3/3/25/25	15/37/135/135	-
19	CLA	AA	837	-	3/3/20/25	0/11/111/135	-
19	CLA	AA	838	-	3/3/19/25	4/11/110/135	-
19	CLA	AA	839	-	3/3/22/25	8/22/120/135	-
19	CLA	AA	840	-	3/3/23/25	7/27/125/135	-
19	CLA	AA	841	-	3/3/20/25	4/15/113/135	-
19	CLA	AA	842	-	3/3/25/25	10/37/135/135	-
19	CLA	AA	843	-	3/3/25/25	15/37/135/135	-
21	PQN	AA	844	-	-	4/23/43/43	0/2/2/2
19	CLA	AA	845	-	3/3/19/25	3/8/106/135	-
22	LHG	AA	846	-	-	20/53/53/53	-
22	LHG	AA	847	-	-	12/42/42/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	AA	848	-	-	13/27/61/63	0/2/2/2
23	BCR	AA	849	-	-	19/29/63/63	0/2/2/2
23	BCR	AA	850	-	-	16/29/63/63	0/2/2/2
23	BCR	AA	851	-	-	15/29/63/63	0/2/2/2
23	BCR	AA	852	-	-	19/29/63/63	0/2/2/2
19	CLA	AA	853	-	3/3/25/25	18/37/135/135	-
23	BCR	AA	854	-	-	18/29/63/63	0/2/2/2
23	BCR	AA	855	-	-	18/29/63/63	0/2/2/2
24	AJP	AA	856	-	-	2/4/99/220	0/6/6/11
19	CLA	B	801	-	3/3/25/25	17/37/135/135	-
19	CLA	B	802	-	3/3/25/25	11/37/135/135	-
19	CLA	B	803	-	3/3/25/25	13/37/135/135	-
19	CLA	B	804	-	3/3/24/25	8/34/132/135	-
19	CLA	B	805	-	3/3/24/25	9/36/134/135	-
19	CLA	B	806	-	3/3/25/25	15/37/135/135	-
19	CLA	B	807	-	3/3/25/25	11/37/135/135	-
19	CLA	B	808	-	3/3/24/25	10/31/129/135	-
19	CLA	B	809	-	3/3/20/25	4/11/111/135	-
19	CLA	B	810	-	3/3/25/25	15/37/135/135	-
19	CLA	B	811	-	3/3/24/25	15/33/131/135	-
19	CLA	B	812	-	3/3/19/25	4/8/106/135	-
19	CLA	B	813	-	3/3/19/25	6/10/108/135	-
19	CLA	B	814	-	3/3/23/25	10/30/128/135	-
19	CLA	B	815	-	3/3/25/25	18/37/135/135	-
19	CLA	B	816	-	3/3/23/25	9/28/126/135	-
19	CLA	B	817	-	3/3/19/25	3/10/108/135	-
19	CLA	B	818	-	3/3/19/25	4/8/106/135	-
19	CLA	B	819	-	3/3/19/25	2/8/106/135	-
19	CLA	B	820	-	3/3/20/25	7/11/111/135	-
19	CLA	B	821	2	3/3/25/25	14/37/135/135	-
19	CLA	B	822	-	3/3/25/25	4/37/135/135	-
19	CLA	B	823	-	3/3/25/25	14/37/135/135	-
19	CLA	B	824	-	3/3/23/25	12/25/123/135	-
19	CLA	B	825	-	3/3/25/25	20/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	826	-	3/3/25/25	14/37/135/135	-
19	CLA	B	827	-	3/3/20/25	6/11/111/135	-
19	CLA	B	828	-	3/3/20/25	2/11/111/135	-
19	CLA	B	829	-	3/3/25/25	13/37/135/135	-
19	CLA	B	830	-	3/3/23/25	4/27/125/135	-
19	CLA	B	831	-	3/3/23/25	5/27/125/135	-
19	CLA	B	832	-	3/3/20/25	4/11/111/135	-
19	CLA	B	833	-	2/2/25/25	12/37/135/135	-
19	CLA	B	834	-	3/3/24/25	18/37/135/135	-
19	CLA	B	835	-	3/3/20/25	1/11/111/135	-
19	CLA	B	836	-	3/3/25/25	9/37/135/135	-
19	CLA	B	837	-	3/3/24/25	10/31/129/135	-
21	PQN	B	838	-	-	7/23/43/43	0/2/2/2
23	BCR	B	839	-	-	16/29/63/63	0/2/2/2
23	BCR	B	840	-	-	9/29/63/63	0/2/2/2
26	ECH	B	841	-	-	16/29/66/66	0/2/2/2
23	BCR	B	842	-	-	19/29/63/63	0/2/2/2
23	BCR	B	843	-	-	16/29/63/63	0/2/2/2
23	BCR	B	844	-	-	15/29/63/63	0/2/2/2
25	LMG	B	845	-	-	19/50/70/70	0/1/1/1
19	CLA	B	846	-	3/3/17/25	1/5/99/135	-
23	BCR	B	848	-	-	17/29/63/63	0/2/2/2
24	AJP	B	849	-	8/8/19/38	3/6/121/220	0/7/7/11
24	AJP	B	850	-	7/7/19/38	2/6/121/220	0/7/7/11
25	LMG	B	851	-	-	17/50/70/70	0/1/1/1
22	LHG	B	852	-	-	13/37/37/53	-
22	LHG	B	853	-	-	23/53/53/53	-
19	CLA	B	854	-	3/3/25/25	13/37/135/135	-
28	DGD	B	856	-	-	21/31/71/95	0/2/2/2
24	AJP	B	857	-	-	0/6/121/220	0/7/7/11
19	CLA	B	858	-	3/3/25/25	5/37/135/135	-
19	CLA	B	859	-	3/3/24/25	13/31/129/135	-
19	CLA	B	860	-	3/3/25/25	15/37/135/135	-
27	SF4	B	861	-	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B1	801	-	3/3/25/25	20/37/135/135	-
19	CLA	B1	802	-	3/3/25/25	14/37/135/135	-
19	CLA	B1	803	-	3/3/25/25	13/37/135/135	-
19	CLA	B1	804	-	3/3/24/25	10/34/132/135	-
19	CLA	B1	805	-	3/3/24/25	9/36/134/135	-
19	CLA	B1	806	-	3/3/25/25	15/37/135/135	-
19	CLA	B1	807	-	3/3/25/25	11/37/135/135	-
19	CLA	B1	808	-	3/3/24/25	11/31/129/135	-
19	CLA	B1	809	-	3/3/20/25	4/11/111/135	-
19	CLA	B1	810	-	3/3/25/25	16/37/135/135	-
19	CLA	B1	811	-	3/3/24/25	15/33/131/135	-
19	CLA	B1	812	-	3/3/19/25	6/8/106/135	-
19	CLA	B1	813	-	3/3/19/25	6/10/108/135	-
19	CLA	B1	814	-	3/3/23/25	12/30/128/135	-
19	CLA	B1	815	-	3/3/25/25	16/37/135/135	-
19	CLA	B1	816	-	3/3/23/25	9/28/126/135	-
19	CLA	B1	817	-	3/3/19/25	2/10/108/135	-
19	CLA	B1	818	-	3/3/19/25	2/8/106/135	-
19	CLA	B1	819	-	3/3/19/25	3/8/106/135	-
19	CLA	B1	820	-	3/3/20/25	7/11/111/135	-
19	CLA	B1	821	2	3/3/25/25	14/37/135/135	-
19	CLA	B1	822	-	3/3/25/25	2/37/135/135	-
19	CLA	B1	823	-	3/3/25/25	16/37/135/135	-
19	CLA	B1	824	-	3/3/23/25	13/25/123/135	-
19	CLA	B1	825	-	3/3/25/25	18/37/135/135	-
19	CLA	B1	826	-	3/3/25/25	15/37/135/135	-
19	CLA	B1	827	-	3/3/20/25	6/11/111/135	-
19	CLA	B1	828	-	3/3/25/25	11/37/135/135	-
19	CLA	B1	829	-	3/3/23/25	5/27/125/135	-
19	CLA	B1	830	-	3/3/23/25	8/27/125/135	-
19	CLA	B1	831	-	3/3/20/25	4/11/111/135	-
19	CLA	B1	832	-	3/3/25/25	12/37/135/135	-
19	CLA	B1	833	-	3/3/24/25	18/37/135/135	-
19	CLA	B1	834	-	3/3/20/25	1/11/111/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B1	835	-	3/3/25/25	10/37/135/135	-
19	CLA	B1	836	-	3/3/24/25	10/31/129/135	-
21	PQN	B1	837	-	-	7/23/43/43	0/2/2/2
23	BCR	B1	838	-	-	19/29/63/63	0/2/2/2
23	BCR	B1	839	-	-	9/29/63/63	0/2/2/2
26	ECH	B1	840	-	-	16/29/66/66	0/2/2/2
23	BCR	B1	841	-	-	19/29/63/63	0/2/2/2
23	BCR	B1	842	-	-	16/29/63/63	0/2/2/2
23	BCR	B1	843	-	-	13/29/63/63	0/2/2/2
25	LMG	B1	844	-	-	20/50/70/70	0/1/1/1
19	CLA	B1	845	-	3/3/17/25	0/5/99/135	-
25	LMG	B1	846	-	-	10/27/47/70	0/1/1/1
22	LHG	B1	847	-	-	14/37/37/53	-
19	CLA	B1	848	-	3/3/25/25	16/37/135/135	-
19	CLA	B1	849	-	3/3/25/25	4/37/135/135	-
19	CLA	B1	850	-	3/3/24/25	10/31/129/135	-
27	SF4	B1	851	-	-	-	0/6/5/5
25	LMG	B1	852	-	-	5/25/45/70	0/1/1/1
19	CLA	B2	801	-	3/3/25/25	18/37/135/135	-
19	CLA	B2	802	-	3/3/25/25	9/37/135/135	-
19	CLA	B2	803	-	3/3/25/25	13/37/135/135	-
19	CLA	B2	804	-	3/3/24/25	9/34/132/135	-
19	CLA	B2	805	-	3/3/24/25	9/36/134/135	-
19	CLA	B2	806	2	3/3/25/25	15/37/135/135	-
19	CLA	B2	807	-	3/3/25/25	14/37/135/135	-
19	CLA	B2	808	-	3/3/24/25	11/31/129/135	-
19	CLA	B2	809	-	3/3/20/25	4/11/111/135	-
19	CLA	B2	810	-	3/3/25/25	16/37/135/135	-
19	CLA	B2	811	-	3/3/24/25	15/33/131/135	-
19	CLA	B2	812	-	3/3/19/25	4/8/106/135	-
19	CLA	B2	813	-	3/3/19/25	6/10/108/135	-
19	CLA	B2	814	-	3/3/23/25	12/30/128/135	-
19	CLA	B2	815	-	3/3/25/25	15/37/135/135	-
19	CLA	B2	816	-	3/3/23/25	8/28/126/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B2	817	-	3/3/19/25	2/10/108/135	-
19	CLA	B2	818	-	3/3/19/25	2/8/106/135	-
19	CLA	B2	819	-	3/3/19/25	3/8/106/135	-
19	CLA	B2	820	-	3/3/20/25	8/11/111/135	-
19	CLA	B2	821	-	3/3/25/25	14/37/135/135	-
19	CLA	B2	822	-	3/3/25/25	7/37/135/135	-
19	CLA	B2	823	-	3/3/25/25	17/37/135/135	-
19	CLA	B2	824	-	3/3/23/25	13/25/123/135	-
19	CLA	B2	825	-	3/3/25/25	20/37/135/135	-
19	CLA	B2	826	-	3/3/25/25	16/37/135/135	-
19	CLA	B2	827	-	3/3/20/25	4/11/111/135	-
19	CLA	B2	828	-	3/3/20/25	1/11/111/135	-
19	CLA	B2	829	-	3/3/25/25	13/37/135/135	-
19	CLA	B2	830	-	3/3/23/25	4/27/125/135	-
19	CLA	B2	831	-	3/3/23/25	9/27/125/135	-
19	CLA	B2	832	-	3/3/20/25	4/11/111/135	-
19	CLA	B2	833	-	2/2/25/25	11/37/135/135	-
19	CLA	B2	834	-	3/3/24/25	20/37/135/135	-
19	CLA	B2	835	-	3/3/20/25	2/11/111/135	-
19	CLA	B2	836	-	3/3/25/25	11/37/135/135	-
19	CLA	B2	837	-	3/3/24/25	10/31/129/135	-
21	PQN	B2	838	-	-	7/23/43/43	0/2/2/2
23	BCR	B2	839	-	-	19/29/63/63	0/2/2/2
23	BCR	B2	840	-	-	8/29/63/63	0/2/2/2
26	ECH	B2	841	-	-	16/29/66/66	0/2/2/2
23	BCR	B2	842	-	-	21/29/63/63	0/2/2/2
23	BCR	B2	843	-	-	18/29/63/63	0/2/2/2
23	BCR	B2	844	-	-	13/29/63/63	0/2/2/2
25	LMG	B2	845	-	-	21/50/70/70	0/1/1/1
19	CLA	B2	846	-	3/3/17/25	0/5/99/135	-
25	LMG	B2	847	-	-	9/27/47/70	0/1/1/1
22	LHG	B2	848	-	-	9/37/37/53	-
19	CLA	B2	849	-	3/3/25/25	14/37/135/135	-
19	CLA	B2	850	-	3/3/25/25	4/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B2	851	-	3/3/24/25	11/31/129/135	-
19	CLA	B2	852	-	3/3/25/25	15/37/135/135	-
27	SF4	B2	853	-	-	-	0/6/5/5
25	LMG	B2	854	-	-	5/25/45/70	0/1/1/1
19	CLA	BB	801	-	3/3/25/25	20/37/135/135	-
19	CLA	BB	802	-	3/3/25/25	16/37/135/135	-
19	CLA	BB	803	-	3/3/25/25	14/37/135/135	-
19	CLA	BB	804	-	3/3/24/25	9/34/132/135	-
19	CLA	BB	805	-	3/3/24/25	9/36/134/135	-
19	CLA	BB	806	-	3/3/25/25	15/37/135/135	-
19	CLA	BB	807	-	3/3/25/25	11/37/135/135	-
19	CLA	BB	808	-	3/3/24/25	13/31/129/135	-
19	CLA	BB	809	-	3/3/20/25	4/11/111/135	-
19	CLA	BB	810	-	3/3/25/25	16/37/135/135	-
19	CLA	BB	811	-	3/3/24/25	17/33/131/135	-
19	CLA	BB	812	-	3/3/19/25	6/8/106/135	-
19	CLA	BB	813	-	3/3/19/25	6/10/108/135	-
19	CLA	BB	814	-	3/3/23/25	11/30/128/135	-
19	CLA	BB	815	-	3/3/25/25	17/37/135/135	-
19	CLA	BB	816	-	3/3/23/25	8/28/126/135	-
19	CLA	BB	817	-	3/3/19/25	1/10/108/135	-
19	CLA	BB	818	-	3/3/19/25	2/8/106/135	-
19	CLA	BB	819	-	3/3/19/25	2/8/106/135	-
19	CLA	BB	820	-	3/3/20/25	8/11/111/135	-
19	CLA	BB	821	-	3/3/25/25	17/37/135/135	-
19	CLA	BB	822	-	3/3/25/25	8/37/135/135	-
19	CLA	BB	823	-	3/3/25/25	14/37/135/135	-
19	CLA	BB	824	-	3/3/23/25	12/25/123/135	-
19	CLA	BB	825	-	3/3/25/25	20/37/135/135	-
19	CLA	BB	826	-	3/3/25/25	17/37/135/135	-
19	CLA	BB	827	-	3/3/20/25	2/11/111/135	-
19	CLA	BB	828	-	3/3/20/25	1/11/111/135	-
19	CLA	BB	829	-	3/3/23/25	6/27/125/135	-
19	CLA	BB	830	-	3/3/23/25	8/27/125/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	BB	831	-	3/3/20/25	4/11/111/135	-
19	CLA	BB	832	-	2/2/25/25	12/37/135/135	-
19	CLA	BB	833	-	3/3/24/25	16/37/135/135	-
19	CLA	BB	834	-	3/3/20/25	1/11/111/135	-
19	CLA	BB	835	-	3/3/25/25	9/37/135/135	-
19	CLA	BB	836	-	3/3/24/25	10/31/129/135	-
21	PQN	BB	837	-	-	7/23/43/43	0/2/2/2
23	BCR	BB	838	-	-	15/29/63/63	0/2/2/2
23	BCR	BB	839	-	-	9/29/63/63	0/2/2/2
26	ECH	BB	840	-	-	15/29/66/66	0/2/2/2
23	BCR	BB	841	-	-	20/29/63/63	0/2/2/2
23	BCR	BB	842	-	-	16/29/63/63	0/2/2/2
23	BCR	BB	843	-	-	13/29/63/63	0/2/2/2
25	LMG	BB	844	-	-	18/50/70/70	0/1/1/1
19	CLA	BB	845	-	3/3/17/25	1/5/99/135	-
23	BCR	BB	847	-	-	17/29/63/63	0/2/2/2
24	AJP	BB	848	-	7/7/19/38	3/6/121/220	0/7/7/11
24	AJP	BB	849	-	7/7/19/38	3/6/121/220	0/7/7/11
22	LHG	BB	850	-	-	14/37/37/53	-
22	LHG	BB	851	-	-	20/53/53/53	-
19	CLA	BB	852	-	3/3/25/25	13/37/135/135	-
28	DGD	BB	854	-	-	21/31/71/95	0/2/2/2
19	CLA	BB	855	-	3/3/25/25	6/37/135/135	-
19	CLA	BB	856	-	3/3/24/25	13/31/129/135	-
27	SF4	BB	857	-	-	-	0/6/5/5
27	SF4	C	101	-	-	-	0/6/5/5
27	SF4	C	102	3	-	-	0/6/5/5
27	SF4	C1	101	-	-	-	0/6/5/5
27	SF4	C1	102	-	-	-	0/6/5/5
27	SF4	C2	101	-	-	-	0/6/5/5
27	SF4	C2	102	-	-	-	0/6/5/5
27	SF4	CC	101	-	-	-	0/6/5/5
27	SF4	CC	102	-	-	-	0/6/5/5
19	CLA	F	301	-	3/3/24/25	12/31/129/135	-
19	CLA	F	302	-	3/3/19/25	4/10/108/135	-
23	BCR	F	303	-	-	18/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	F	304	-	-	15/29/63/63	0/2/2/2
23	BCR	F	305	-	-	23/29/63/63	0/2/2/2
19	CLA	F1	301	-	3/3/24/25	11/31/129/135	-
19	CLA	F1	302	-	3/3/19/25	4/10/108/135	-
23	BCR	F1	303	-	-	17/29/63/63	0/2/2/2
23	BCR	F1	304	-	-	15/29/63/63	0/2/2/2
19	CLA	F1	305	-	3/3/20/25	2/11/111/135	-
23	BCR	F1	306	-	-	25/29/63/63	0/2/2/2
19	CLA	F2	301	-	3/3/24/25	11/31/129/135	-
19	CLA	F2	302	-	3/3/19/25	4/10/108/135	-
23	BCR	F2	303	-	-	20/29/63/63	0/2/2/2
23	BCR	F2	304	-	-	15/29/63/63	0/2/2/2
23	BCR	F2	305	-	-	26/29/63/63	0/2/2/2
19	CLA	FF	301	-	3/3/24/25	13/31/129/135	-
19	CLA	FF	302	-	3/3/19/25	4/10/108/135	-
23	BCR	FF	303	-	-	19/29/63/63	0/2/2/2
23	BCR	FF	304	-	-	14/29/63/63	0/2/2/2
19	CLA	FF	305	-	3/3/25/25	11/37/135/135	-
23	BCR	FF	306	-	-	22/29/63/63	0/2/2/2
23	BCR	I	101	-	-	20/29/63/63	0/2/2/2
23	BCR	I	102	-	-	10/29/63/63	0/2/2/2
23	BCR	I1	101	-	-	18/29/63/63	0/2/2/2
25	LMG	I1	102	-	-	18/30/50/70	0/1/1/1
23	BCR	I2	101	-	-	17/29/63/63	0/2/2/2
23	BCR	I2	102	-	-	11/29/63/63	0/2/2/2
23	BCR	I2	103	-	-	18/29/63/63	0/2/2/2
24	AJP	I2	104	-	3/3/14/38	-	0/6/6/11
25	LMG	I2	105	-	-	10/29/49/70	0/1/1/1
23	BCR	II	101	-	-	17/29/63/63	0/2/2/2
23	BCR	II	102	-	-	9/29/63/63	0/2/2/2
23	BCR	II	104	-	-	18/29/63/63	0/2/2/2
25	LMG	II	105	-	-	20/37/57/70	0/1/1/1
19	CLA	J	101	8	3/3/19/25	3/8/106/135	-
23	BCR	J	102	-	-	19/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	J	103	-	2/2/19/25	6/8/106/135	-
23	BCR	J	104	-	-	16/29/63/63	0/2/2/2
19	CLA	J1	101	-	3/3/18/25	3/8/106/135	-
23	BCR	J1	102	-	-	19/29/63/63	0/2/2/2
19	CLA	J1	103	-	3/3/19/25	0/8/106/135	-
23	BCR	J1	104	-	-	18/29/63/63	0/2/2/2
19	CLA	J2	101	8	3/3/19/25	3/8/106/135	-
23	BCR	J2	102	-	-	18/29/63/63	0/2/2/2
19	CLA	J2	103	-	3/3/19/25	0/8/106/135	-
23	BCR	J2	104	-	-	16/29/63/63	0/2/2/2
19	CLA	JJ	101	8	3/3/19/25	3/8/106/135	-
23	BCR	JJ	102	-	-	20/29/63/63	0/2/2/2
19	CLA	JJ	103	-	3/3/19/25	0/8/106/135	-
23	BCR	JJ	104	-	-	16/29/63/63	0/2/2/2
19	CLA	K	101	-	3/3/20/25	1/11/111/135	-
19	CLA	K	102	-	3/3/20/25	11/15/113/135	-
23	BCR	K	103	-	-	19/29/63/63	0/2/2/2
24	AJP	K	104	-	6/6/19/38	2/4/116/220	0/7/7/11
19	CLA	K1	102	-	3/3/20/25	2/11/111/135	-
19	CLA	K1	103	-	3/3/20/25	8/15/113/135	-
23	BCR	K1	104	-	-	18/29/63/63	0/2/2/2
19	CLA	K1	105	9	3/3/18/25	6/8/102/135	-
23	BCR	K1	106	-	-	17/29/63/63	0/2/2/2
19	CLA	K2	102	-	3/3/20/25	1/11/111/135	-
23	BCR	K2	103	-	-	12/29/63/63	0/2/2/2
19	CLA	K2	104	-	3/3/18/25	2/5/101/135	-
23	BCR	K2	105	-	-	16/29/63/63	0/2/2/2
19	CLA	KK	101	-	3/3/20/25	1/11/111/135	-
19	CLA	KK	102	-	3/3/20/25	10/15/113/135	-
23	BCR	KK	103	-	-	19/29/63/63	0/2/2/2
24	AJP	KK	104	-	6/6/19/38	2/4/116/220	0/7/7/11
19	CLA	L	202	18	3/3/24/25	14/33/131/135	-
19	CLA	L	203	-	3/3/25/25	7/37/135/135	-
19	CLA	L	204	-	3/3/25/25	16/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	L	205	-	-	17/29/63/63	0/2/2/2
23	BCR	L	206	-	-	18/29/63/63	0/2/2/2
22	LHG	L	207	-	-	13/38/38/53	-
24	AJP	L	208	-	4/4/14/38	-	0/6/6/11
24	AJP	L	209	-	4/4/14/38	-	0/6/6/11
23	BCR	L1	201	-	-	12/29/63/63	0/2/2/2
24	AJP	L1	203	-	5/5/19/38	4/6/121/220	0/7/7/11
24	AJP	L1	204	-	5/5/19/38	3/6/121/220	0/7/7/11
19	CLA	L1	205	10	3/3/24/25	11/33/131/135	-
19	CLA	L1	206	-	3/3/25/25	3/37/135/135	-
19	CLA	L1	207	-	3/3/25/25	12/37/135/135	-
23	BCR	L1	208	-	-	17/29/63/63	0/2/2/2
23	BCR	L1	209	-	-	18/29/63/63	0/2/2/2
25	LMG	L1	210	-	-	16/50/70/70	0/1/1/1
22	LHG	L1	211	-	-	13/37/37/53	-
24	AJP	L2	202	-	7/7/19/38	3/6/121/220	0/7/7/11
24	AJP	L2	203	-	6/6/19/38	4/6/121/220	0/7/7/11
19	CLA	L2	204	16	3/3/24/25	15/33/131/135	-
19	CLA	L2	205	-	3/3/23/25	6/30/128/135	-
19	CLA	L2	206	-	3/3/25/25	14/37/135/135	-
23	BCR	L2	207	-	-	19/29/63/63	0/2/2/2
22	LHG	L2	208	-	-	17/39/39/53	-
19	CLA	LL	201	18	3/3/24/25	13/33/131/135	-
19	CLA	LL	202	-	3/3/25/25	6/37/135/135	-
19	CLA	LL	203	-	3/3/19/25	8/10/108/135	-
23	BCR	LL	204	-	-	18/29/63/63	0/2/2/2
22	LHG	LL	205	-	-	13/38/38/53	-
23	BCR	M	101	-	-	22/29/63/63	0/2/2/2
25	LMG	M	102	-	-	15/41/61/70	0/1/1/1
23	BCR	M1	101	-	-	17/29/63/63	0/2/2/2
24	AJP	M2	101	-	3/3/14/38	-	0/6/6/11
23	BCR	M2	102	-	-	18/29/63/63	0/2/2/2
23	BCR	MM	101	-	-	23/29/63/63	0/2/2/2
19	CLA	X	101	-	3/3/20/25	1/11/111/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	LHG	X	102	-	-	18/44/44/53	-
19	CLA	X1	101	-	3/3/20/25	2/11/111/135	-
22	LHG	X1	102	-	-	17/44/44/53	-
22	LHG	X1	103	-	-	19/53/53/53	-
19	CLA	X2	101	-	3/3/20/25	3/11/111/135	-
22	LHG	X2	102	-	-	15/44/44/53	-
22	LHG	X2	103	-	-	22/53/53/53	-
19	CLA	XX	101	-	3/3/20/25	5/11/111/135	-
22	LHG	XX	102	-	-	18/44/44/53	-

The worst 5 of 2620 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	802	AJP	CBL-CCH	-10.99	1.35	1.53
24	AA	802	AJP	CBL-CCH	-10.93	1.35	1.53
24	L	208	AJP	CBL-CCH	-10.78	1.35	1.53
24	BB	849	AJP	CBL-CCH	-10.74	1.35	1.53
24	AA	856	AJP	CCI-CCJ	-10.73	1.39	1.54

The worst 5 of 5097 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A1	854	AJP	CBK-CCG-CCF	-13.21	88.84	108.95
24	B	857	AJP	CBK-CCG-CCF	-13.13	88.97	108.95
24	L1	203	AJP	CBK-CCG-CCF	-13.04	89.10	108.95
24	L2	202	AJP	CBK-CCG-CCF	-12.69	89.64	108.95
24	L	208	AJP	CBK-CCG-CCF	-12.63	89.73	108.95

5 of 1225 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	B2	817	CLA	NC
19	B2	817	CLA	ND
19	B2	817	CLA	NA
19	B1	806	CLA	NC
19	B1	806	CLA	ND

5 of 5794 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	B1	806	CLA	CHA-CBD-CGD-O1D
19	B1	806	CLA	CHA-CBD-CGD-O2D
19	BB	801	CLA	C1A-C2A-CAA-CBA
19	B	834	CLA	C1A-C2A-CAA-CBA
19	B	834	CLA	C4-C3-C5-C6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	855	AJP	CCE-CCF-CCG-CCZ-CDA-CDB

350 monomers are involved in 569 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	801	CLA	1	0
20	A	803	CL0	1	0
19	A	804	CLA	3	0
19	A	805	CLA	3	0
19	A	806	CLA	2	0
19	A	807	CLA	3	0
19	A	809	CLA	1	0
19	A	810	CLA	1	0
19	A	812	CLA	1	0
19	A	813	CLA	1	0
19	A	815	CLA	3	0
19	A	816	CLA	1	0
19	A	818	CLA	1	0
19	A	820	CLA	2	0
19	A	821	CLA	1	0
19	A	822	CLA	3	0
19	A	824	CLA	1	0
19	A	826	CLA	2	0
19	A	828	CLA	1	0
19	A	830	CLA	4	0
19	A	831	CLA	1	0
19	A	832	CLA	3	0
19	A	833	CLA	2	0
19	A	834	CLA	1	0
19	A	836	CLA	1	0
19	A	837	CLA	2	0
19	A	840	CLA	1	0
19	A	841	CLA	1	0
19	A	842	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	843	PQN	3	0
22	A	845	LHG	2	0
22	A	846	LHG	1	0
23	A	847	BCR	1	0
23	A	851	BCR	4	0
19	A	852	CLA	11	0
23	A	854	BCR	2	0
19	A1	801	CLA	1	0
20	A1	802	CL0	3	0
19	A1	803	CLA	3	0
19	A1	804	CLA	2	0
19	A1	805	CLA	2	0
19	A1	806	CLA	4	0
19	A1	807	CLA	1	0
19	A1	811	CLA	2	0
19	A1	812	CLA	1	0
19	A1	814	CLA	4	0
19	A1	815	CLA	2	0
19	A1	816	CLA	1	0
19	A1	817	CLA	2	0
19	A1	819	CLA	2	0
19	A1	820	CLA	3	0
19	A1	822	CLA	1	0
19	A1	824	CLA	1	0
19	A1	826	CLA	1	0
19	A1	827	CLA	1	0
19	A1	828	CLA	3	0
19	A1	829	CLA	3	0
19	A1	830	CLA	1	0
19	A1	831	CLA	2	0
19	A1	832	CLA	1	0
19	A1	833	CLA	2	0
19	A1	834	CLA	2	0
19	A1	835	CLA	1	0
19	A1	836	CLA	1	0
19	A1	839	CLA	2	0
19	A1	840	CLA	1	0
19	A1	841	CLA	3	0
19	A1	842	CLA	1	0
21	A1	843	PQN	1	0
19	A1	844	CLA	1	0
22	A1	846	LHG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A1	847	BCR	2	0
23	A1	850	BCR	1	0
23	A1	851	BCR	3	0
19	A1	852	CLA	11	0
19	A2	801	CLA	1	0
19	A2	802	CLA	1	0
20	A2	803	CL0	5	0
19	A2	804	CLA	3	0
19	A2	805	CLA	3	0
19	A2	806	CLA	3	0
19	A2	807	CLA	2	0
19	A2	812	CLA	1	0
19	A2	813	CLA	1	0
19	A2	815	CLA	4	0
19	A2	816	CLA	1	0
19	A2	818	CLA	2	0
19	A2	820	CLA	1	0
19	A2	821	CLA	4	0
19	A2	825	CLA	1	0
19	A2	826	CLA	1	0
19	A2	828	CLA	1	0
19	A2	829	CLA	1	0
19	A2	830	CLA	2	0
19	A2	831	CLA	1	0
19	A2	832	CLA	2	0
19	A2	833	CLA	2	0
19	A2	834	CLA	1	0
19	A2	835	CLA	1	0
19	A2	836	CLA	1	0
19	A2	840	CLA	1	0
19	A2	841	CLA	1	0
19	A2	842	CLA	4	0
21	A2	843	PQN	1	0
19	A2	844	CLA	1	0
22	A2	845	LHG	1	0
22	A2	846	LHG	1	0
23	A2	847	BCR	1	0
23	A2	850	BCR	1	0
23	A2	851	BCR	5	0
19	A2	852	CLA	9	0
19	AA	801	CLA	1	0
20	AA	803	CL0	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	AA	804	CLA	3	0
19	AA	805	CLA	2	0
19	AA	806	CLA	2	0
19	AA	807	CLA	3	0
19	AA	810	CLA	1	0
19	AA	813	CLA	1	0
19	AA	815	CLA	3	0
19	AA	816	CLA	1	0
19	AA	818	CLA	2	0
19	AA	820	CLA	1	0
19	AA	821	CLA	3	0
19	AA	822	CLA	2	0
19	AA	825	CLA	1	0
19	AA	826	CLA	4	0
19	AA	828	CLA	3	0
19	AA	830	CLA	5	0
19	AA	831	CLA	1	0
19	AA	832	CLA	1	0
19	AA	833	CLA	1	0
19	AA	836	CLA	1	0
19	AA	842	CLA	2	0
19	AA	843	CLA	1	0
21	AA	844	PQN	3	0
19	AA	845	CLA	1	0
22	AA	846	LHG	2	0
22	AA	847	LHG	1	0
23	AA	848	BCR	1	0
23	AA	851	BCR	1	0
23	AA	852	BCR	4	0
19	AA	853	CLA	6	0
23	AA	854	BCR	1	0
23	AA	855	BCR	1	0
19	B	801	CLA	1	0
19	B	802	CLA	2	0
19	B	804	CLA	2	0
19	B	806	CLA	3	0
19	B	809	CLA	1	0
19	B	810	CLA	2	0
19	B	811	CLA	2	0
19	B	813	CLA	1	0
19	B	815	CLA	1	0
19	B	818	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	820	CLA	5	0
19	B	821	CLA	1	0
19	B	822	CLA	2	0
19	B	823	CLA	1	0
19	B	824	CLA	1	0
19	B	826	CLA	2	0
19	B	827	CLA	1	0
19	B	828	CLA	3	0
19	B	829	CLA	3	0
19	B	830	CLA	4	0
19	B	831	CLA	1	0
19	B	832	CLA	2	0
19	B	833	CLA	7	0
19	B	834	CLA	14	0
19	B	835	CLA	8	0
19	B	836	CLA	2	0
19	B	837	CLA	2	0
21	B	838	PQN	2	0
23	B	839	BCR	2	0
26	B	841	ECH	1	0
23	B	842	BCR	5	0
23	B	843	BCR	4	0
23	B	844	BCR	1	0
24	B	849	AJP	1	0
22	B	852	LHG	1	0
19	B	854	CLA	6	0
28	B	856	DGD	1	0
19	B	858	CLA	3	0
19	B	859	CLA	3	0
19	B	860	CLA	2	0
19	B1	802	CLA	1	0
19	B1	804	CLA	2	0
19	B1	806	CLA	1	0
19	B1	807	CLA	1	0
19	B1	808	CLA	1	0
19	B1	809	CLA	1	0
19	B1	810	CLA	3	0
19	B1	811	CLA	2	0
19	B1	813	CLA	1	0
19	B1	814	CLA	1	0
19	B1	815	CLA	3	0
19	B1	820	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B1	821	CLA	1	0
19	B1	822	CLA	1	0
19	B1	823	CLA	1	0
19	B1	824	CLA	1	0
19	B1	826	CLA	1	0
19	B1	827	CLA	2	0
19	B1	828	CLA	3	0
19	B1	829	CLA	2	0
19	B1	830	CLA	1	0
19	B1	831	CLA	3	0
19	B1	832	CLA	5	0
19	B1	833	CLA	14	0
19	B1	834	CLA	9	0
19	B1	835	CLA	1	0
19	B1	836	CLA	1	0
23	B1	838	BCR	1	0
23	B1	839	BCR	1	0
26	B1	840	ECH	1	0
23	B1	841	BCR	2	0
23	B1	842	BCR	3	0
19	B1	845	CLA	1	0
22	B1	847	LHG	1	0
19	B1	848	CLA	6	0
19	B1	849	CLA	1	0
19	B1	850	CLA	2	0
19	B2	802	CLA	1	0
19	B2	804	CLA	1	0
19	B2	806	CLA	2	0
19	B2	808	CLA	1	0
19	B2	809	CLA	1	0
19	B2	810	CLA	3	0
19	B2	811	CLA	2	0
19	B2	813	CLA	1	0
19	B2	816	CLA	1	0
19	B2	820	CLA	1	0
19	B2	821	CLA	3	0
19	B2	822	CLA	1	0
19	B2	823	CLA	1	0
19	B2	826	CLA	2	0
19	B2	827	CLA	1	0
19	B2	828	CLA	1	0
19	B2	829	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B2	830	CLA	3	0
19	B2	831	CLA	1	0
19	B2	832	CLA	3	0
19	B2	833	CLA	3	0
19	B2	834	CLA	4	0
19	B2	835	CLA	3	0
19	B2	836	CLA	1	0
19	B2	837	CLA	1	0
23	B2	839	BCR	1	0
23	B2	840	BCR	1	0
26	B2	841	ECH	1	0
23	B2	842	BCR	4	0
23	B2	843	BCR	3	0
19	B2	846	CLA	1	0
19	B2	849	CLA	5	0
19	B2	850	CLA	3	0
19	B2	851	CLA	2	0
19	B2	852	CLA	2	0
19	BB	801	CLA	1	0
19	BB	802	CLA	1	0
19	BB	804	CLA	2	0
19	BB	805	CLA	1	0
19	BB	806	CLA	2	0
19	BB	810	CLA	4	0
19	BB	811	CLA	1	0
19	BB	812	CLA	1	0
19	BB	813	CLA	1	0
19	BB	815	CLA	2	0
19	BB	817	CLA	1	0
19	BB	820	CLA	5	0
19	BB	821	CLA	2	0
19	BB	822	CLA	2	0
19	BB	823	CLA	2	0
19	BB	826	CLA	2	0
19	BB	828	CLA	3	0
19	BB	829	CLA	4	0
19	BB	831	CLA	1	0
19	BB	832	CLA	7	0
19	BB	833	CLA	14	0
19	BB	834	CLA	6	0
19	BB	835	CLA	2	0
19	BB	836	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	BB	837	PQN	2	0
23	BB	838	BCR	2	0
26	BB	840	ECH	1	0
23	BB	841	BCR	6	0
23	BB	842	BCR	2	0
24	BB	848	AJP	1	0
19	BB	852	CLA	6	0
28	BB	854	DGD	1	0
19	BB	856	CLA	3	0
27	C	102	SF4	1	0
27	C1	102	SF4	1	0
19	F	301	CLA	3	0
19	F	302	CLA	1	0
23	F	303	BCR	2	0
23	F	305	BCR	6	0
19	F1	301	CLA	3	0
19	F1	302	CLA	1	0
23	F1	303	BCR	2	0
19	F1	305	CLA	2	0
23	F1	306	BCR	5	0
19	F2	301	CLA	3	0
19	F2	302	CLA	1	0
23	F2	303	BCR	2	0
23	F2	305	BCR	5	0
19	FF	301	CLA	3	0
19	FF	302	CLA	1	0
23	FF	303	BCR	3	0
19	FF	305	CLA	3	0
23	FF	306	BCR	4	0
23	I1	101	BCR	1	0
23	I2	103	BCR	1	0
25	I2	105	LMG	1	0
23	J	102	BCR	1	0
19	J	103	CLA	4	0
23	J	104	BCR	1	0
23	J1	102	BCR	1	0
19	J1	103	CLA	1	0
23	J1	104	BCR	1	0
23	J2	102	BCR	1	0
19	J2	103	CLA	2	0
23	J2	104	BCR	2	0
23	JJ	102	BCR	1	0

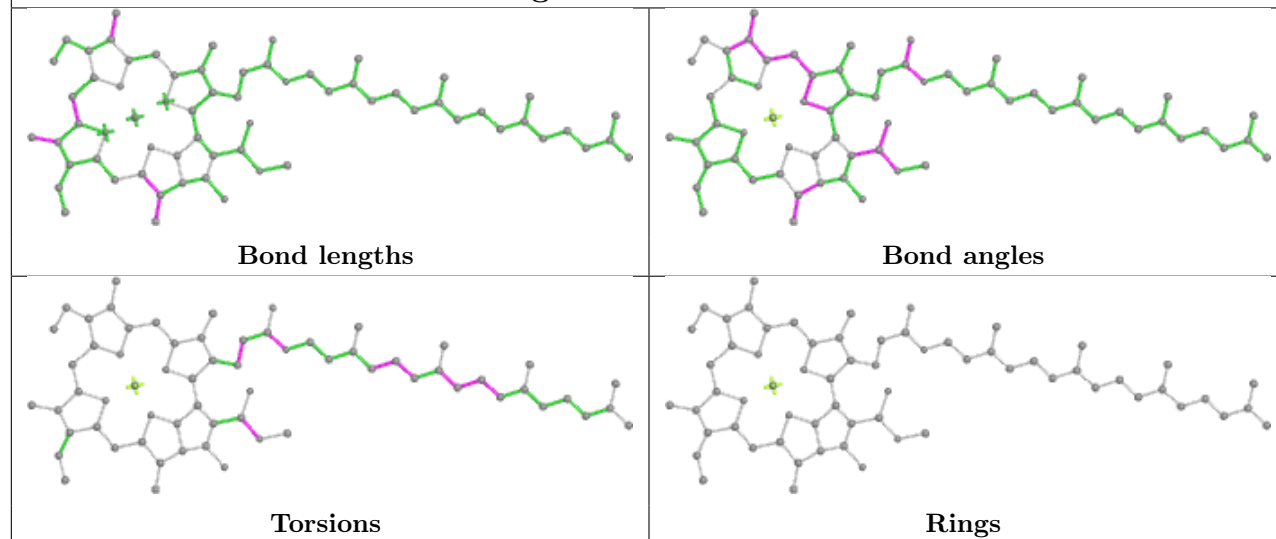
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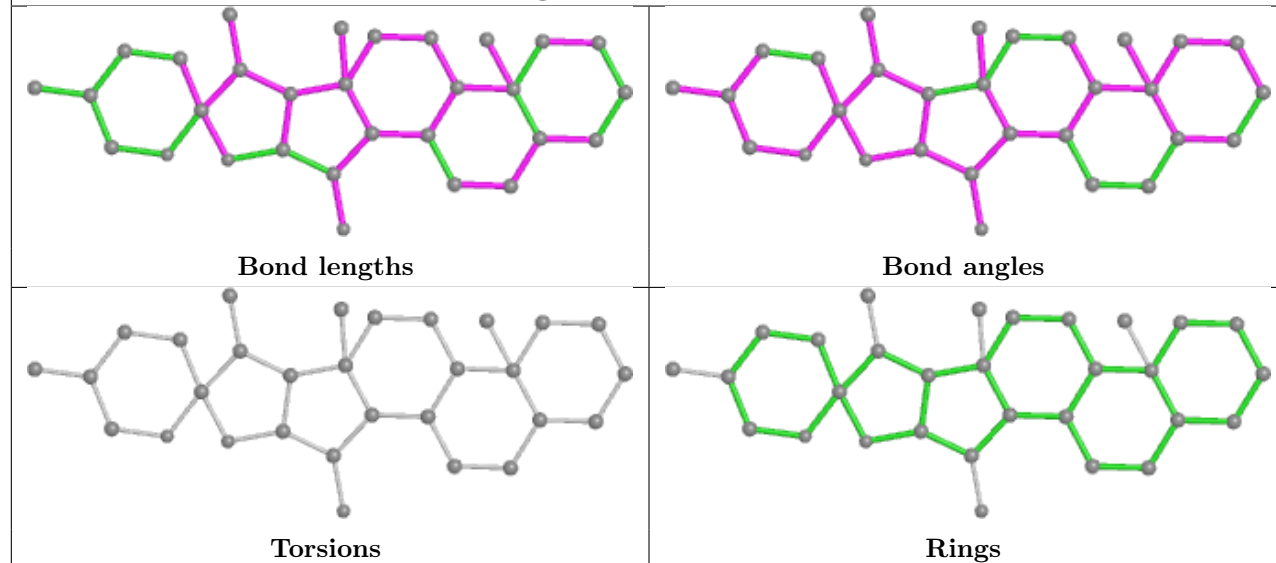
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	JJ	103	CLA	1	0
23	JJ	104	BCR	1	0
19	K1	103	CLA	1	0
23	K1	104	BCR	1	0
19	K1	105	CLA	1	0
23	K1	106	BCR	2	0
23	K2	103	BCR	1	0
19	K2	104	CLA	1	0
23	K2	105	BCR	2	0
19	L	202	CLA	4	0
23	L	205	BCR	1	0
24	L1	204	AJP	1	0
19	L1	205	CLA	3	0
19	L1	206	CLA	1	0
19	L1	207	CLA	1	0
25	L1	210	LMG	1	0
22	L1	211	LHG	3	0
24	L2	203	AJP	1	0
22	L2	208	LHG	2	0
19	LL	201	CLA	5	0
19	LL	202	CLA	1	0
19	LL	203	CLA	1	0
23	LL	204	BCR	1	0
23	M	101	BCR	2	0
25	M	102	LMG	1	0
23	MM	101	BCR	1	0
19	X2	101	CLA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

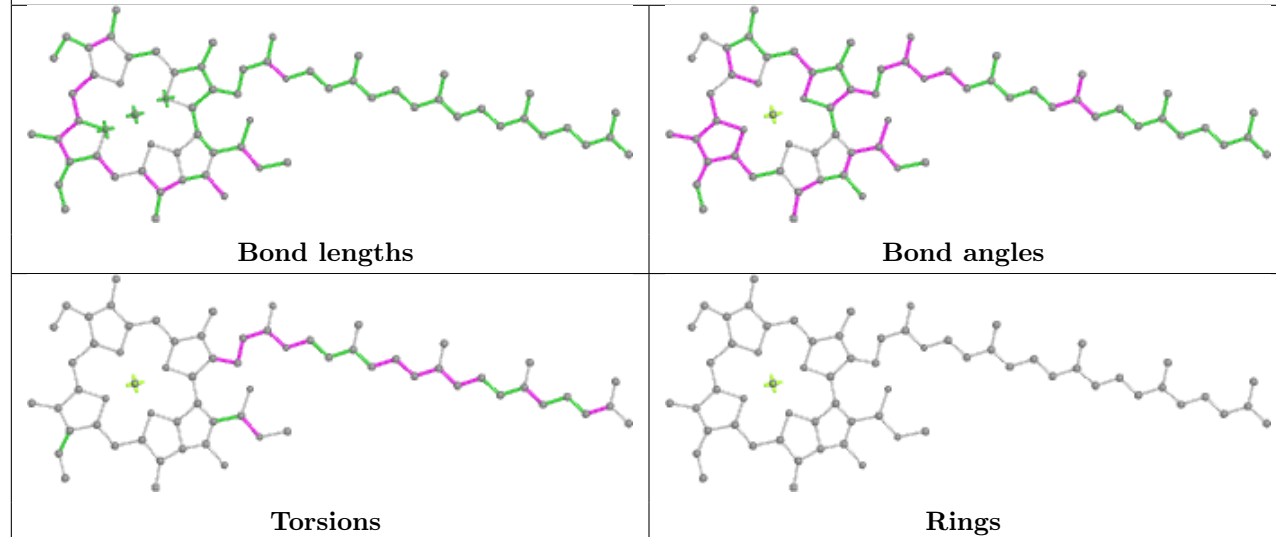
Ligand CLA A 801



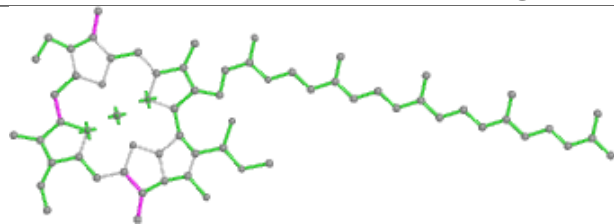
Ligand AJP A 802



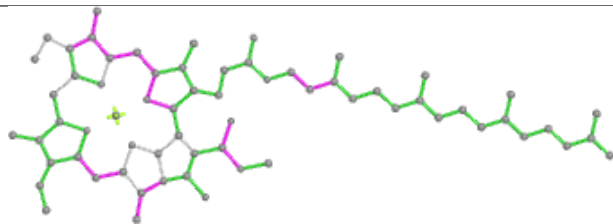
Ligand CL0 A 803



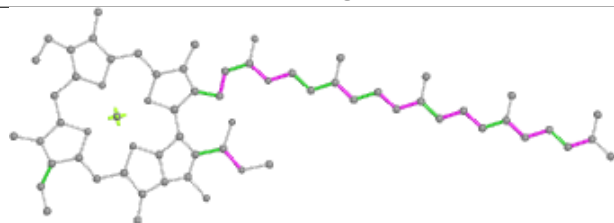
Ligand CLA A 804



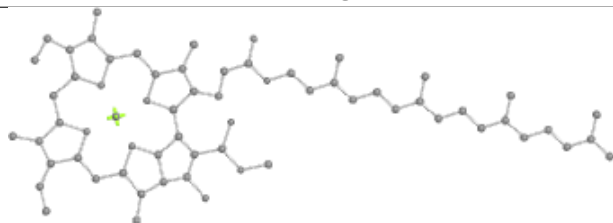
Bond lengths



Bond angles

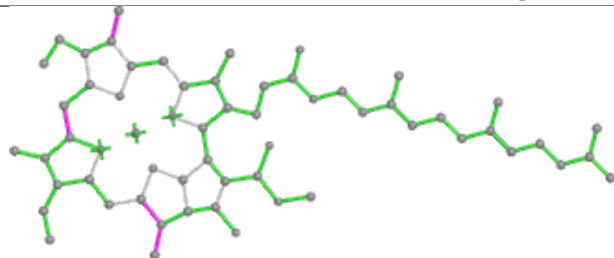


Torsions

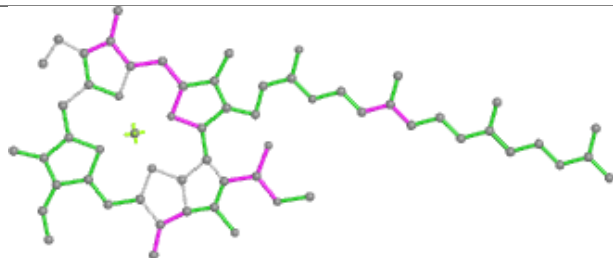


Rings

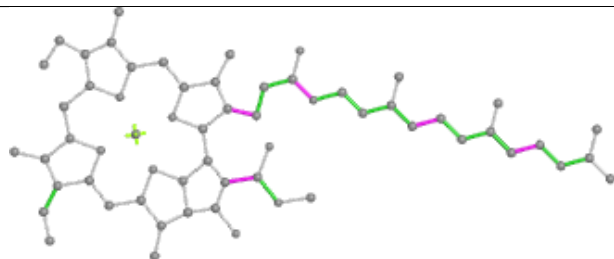
Ligand CLA A 805



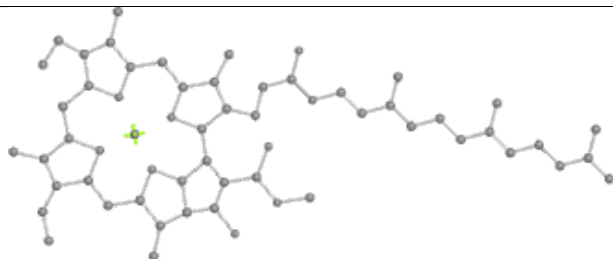
Bond lengths



Bond angles

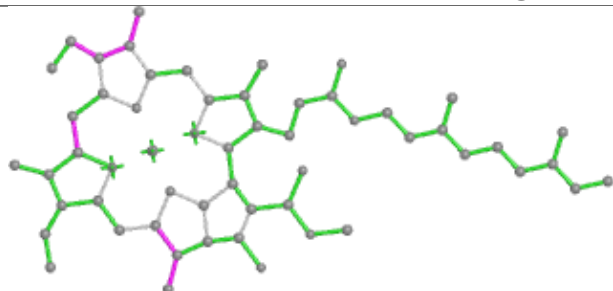


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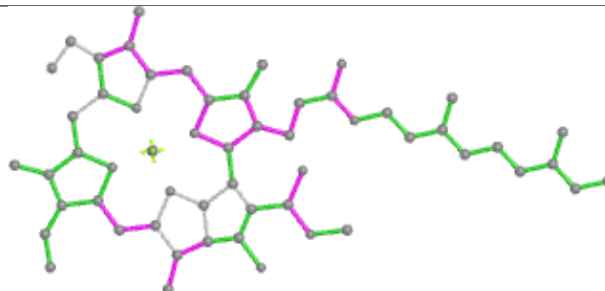


Rings

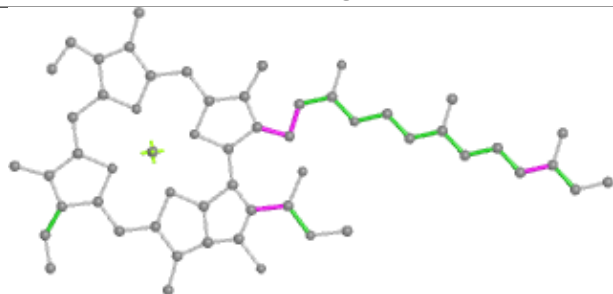
Ligand CLA A 806



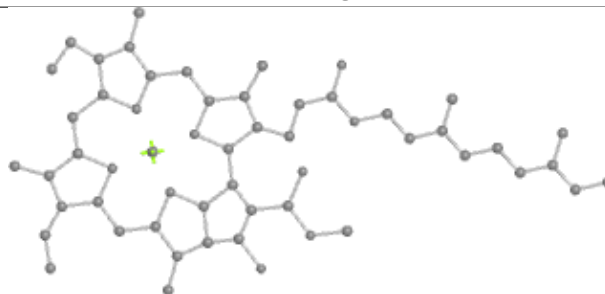
Bond lengths



Bond angles

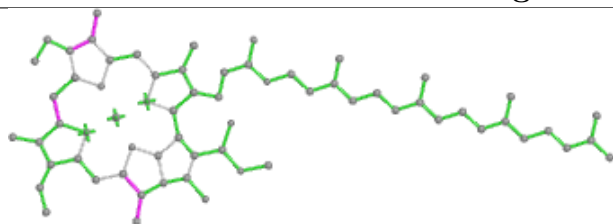


Torsions

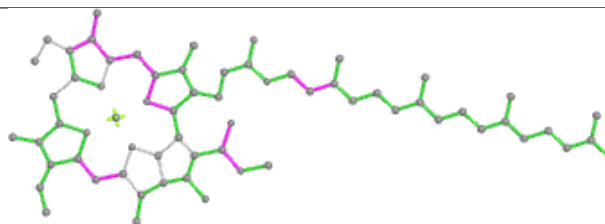


Rings

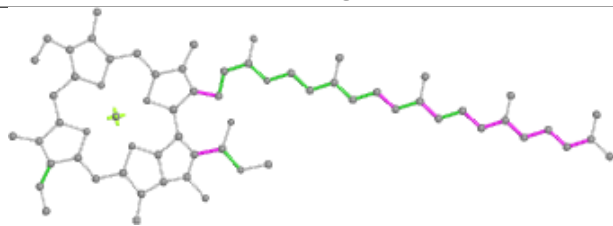
Ligand CLA A 807



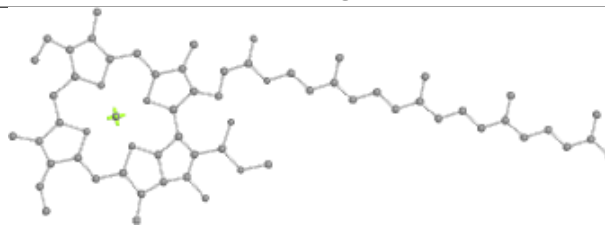
Bond lengths



Bond angles

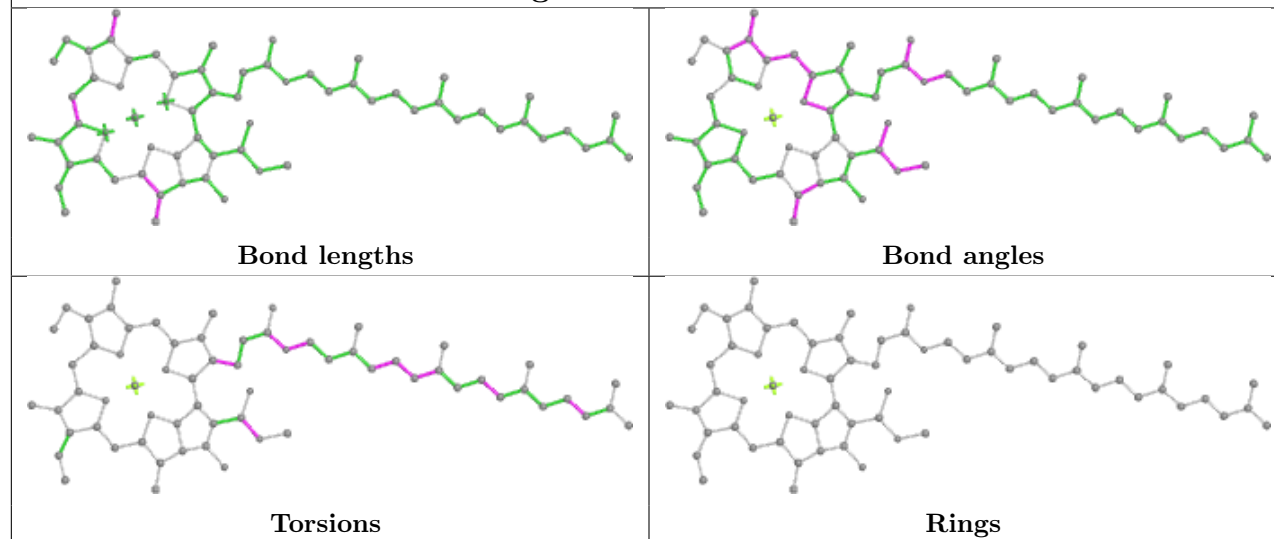


Torsions

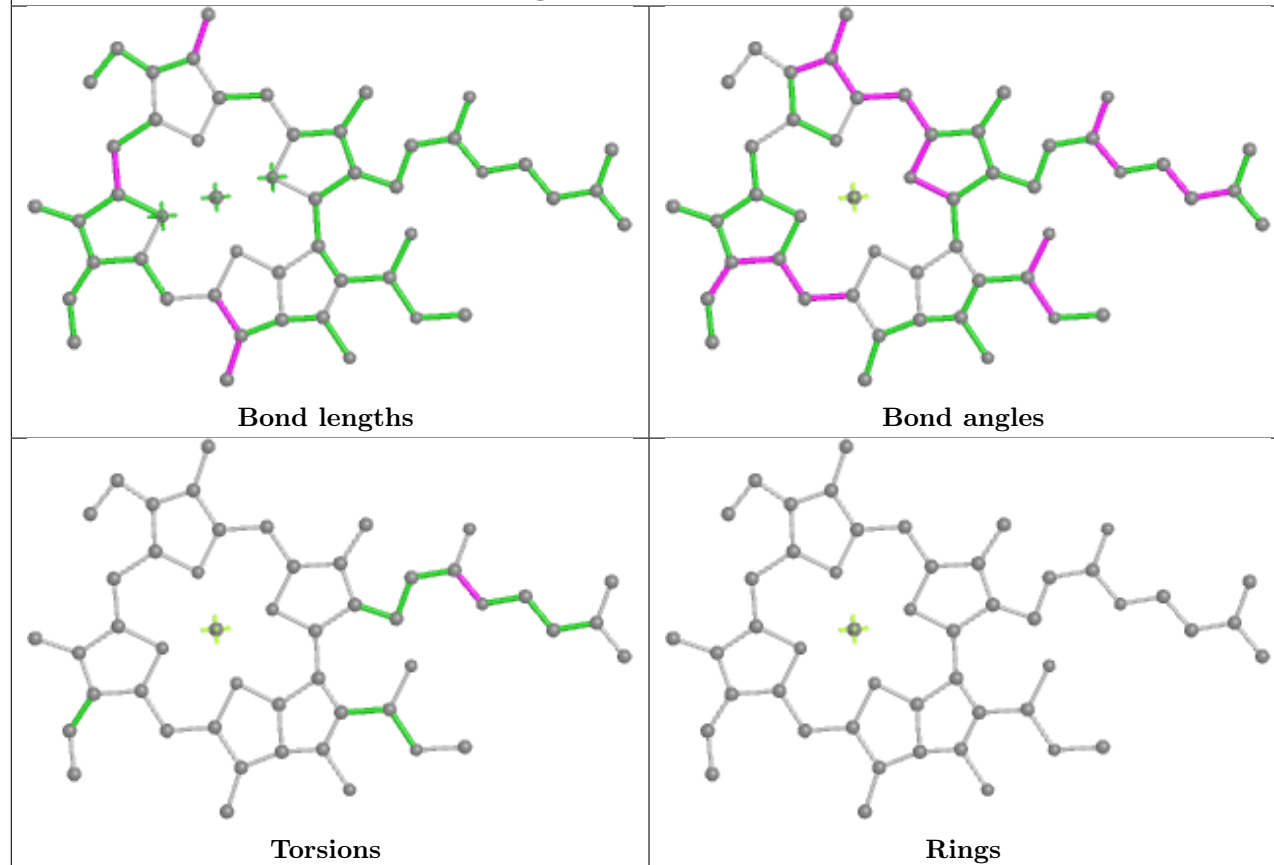


Rings

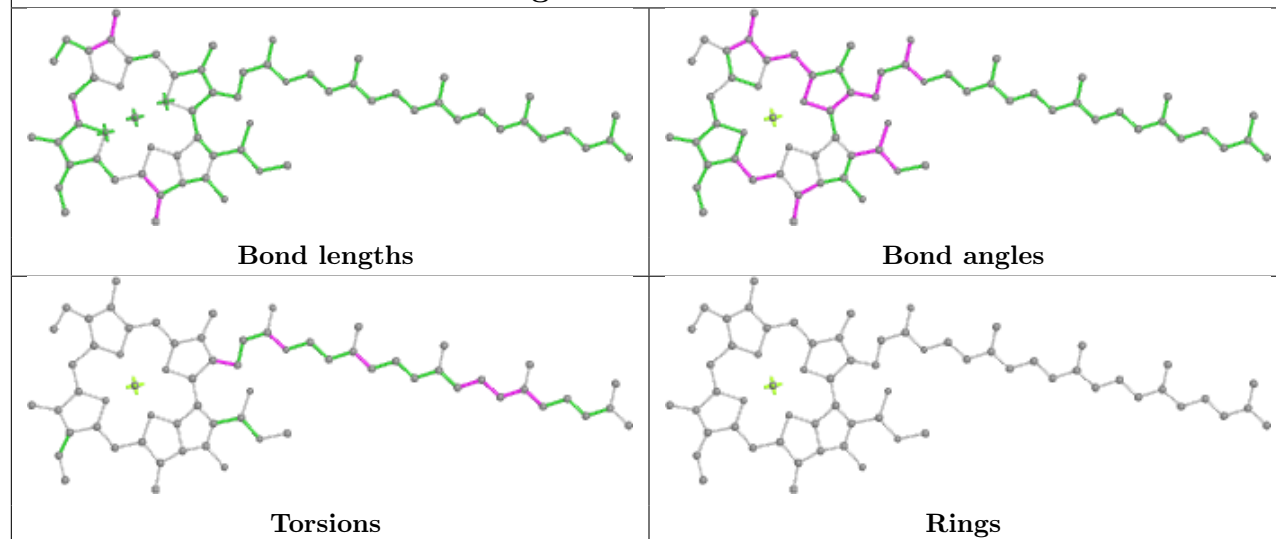
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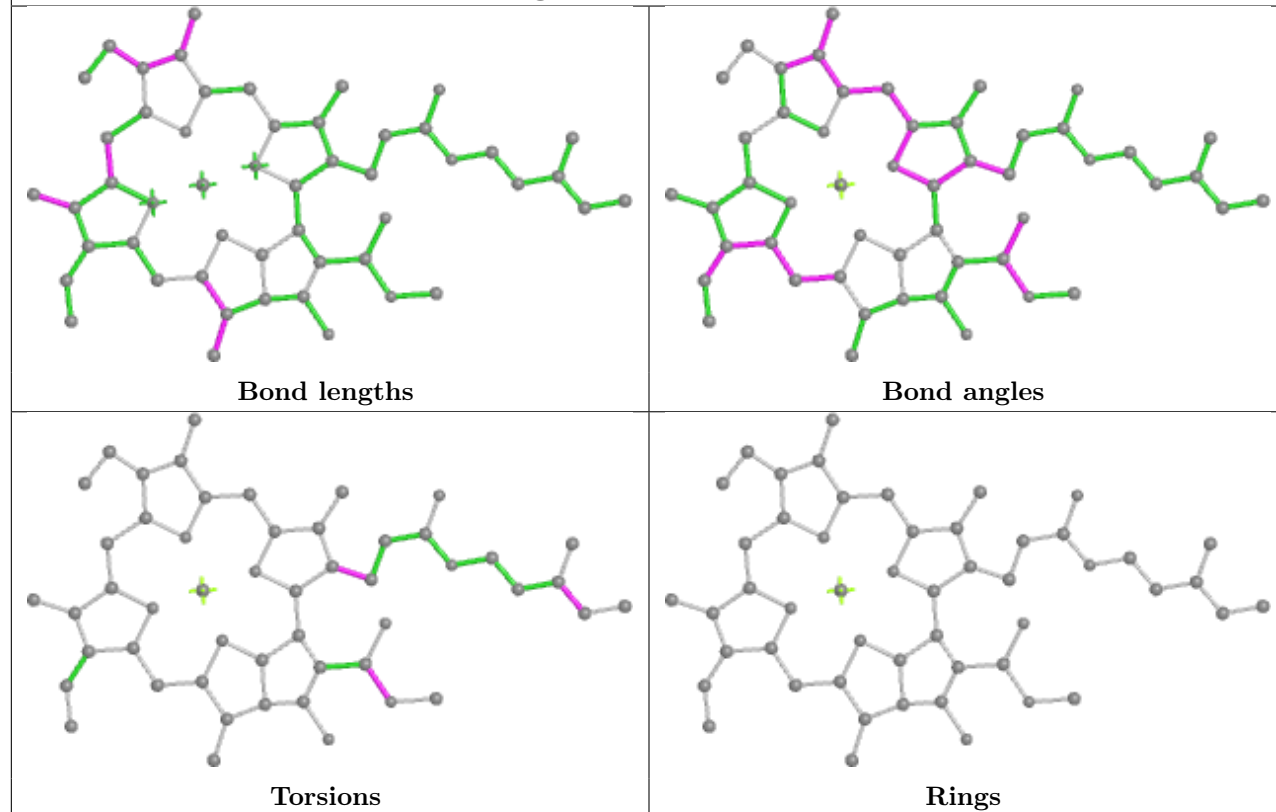
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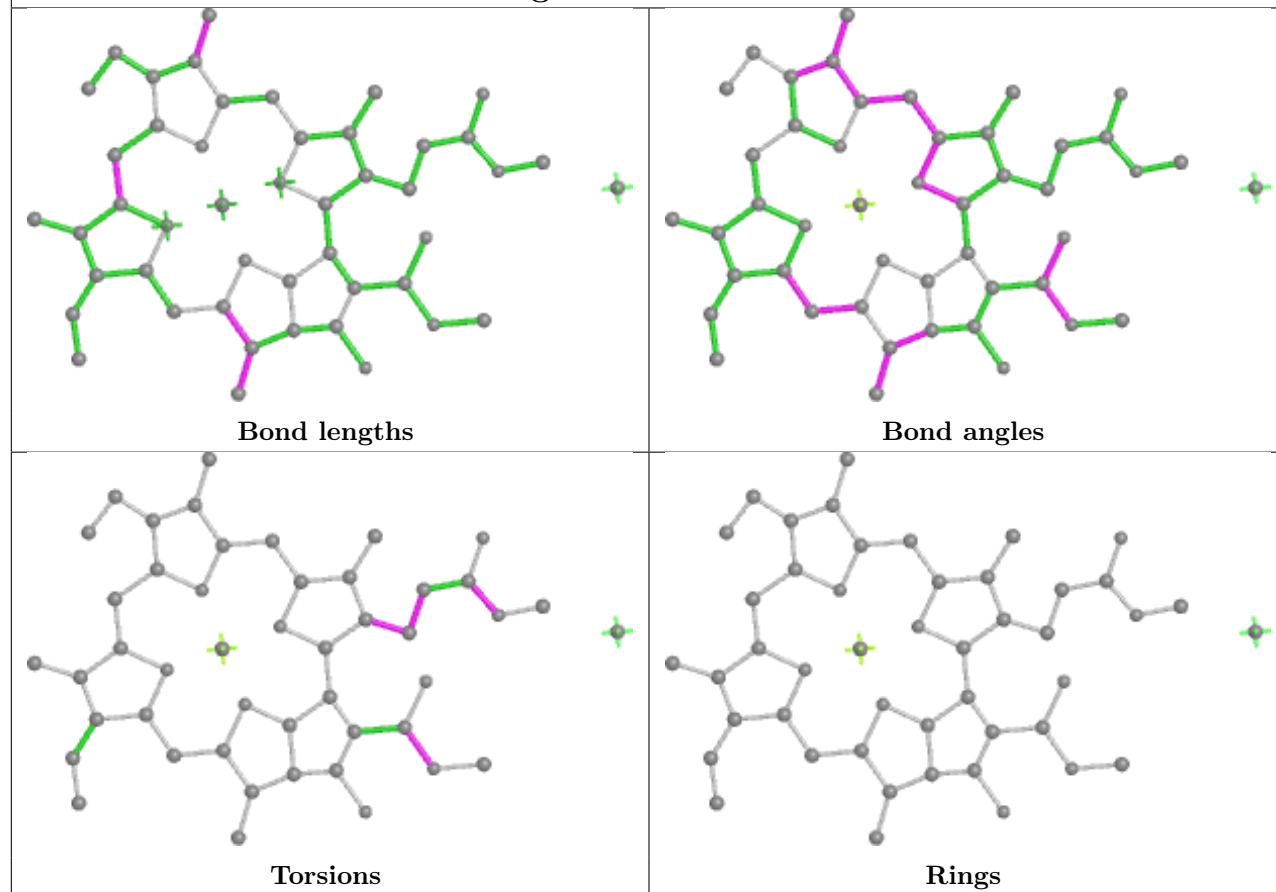
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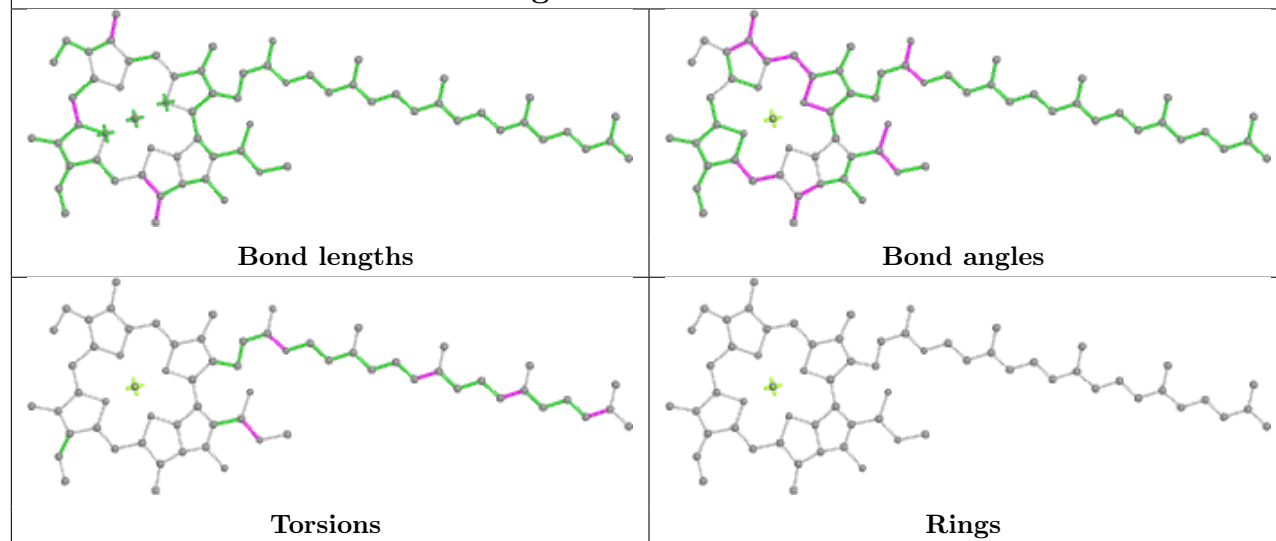
Ligand CLA A 811



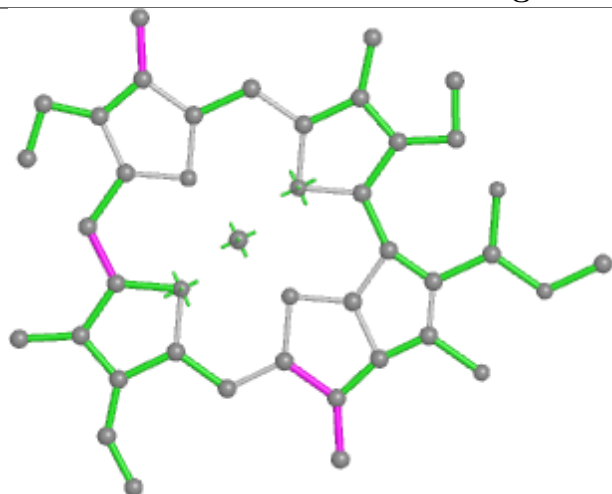
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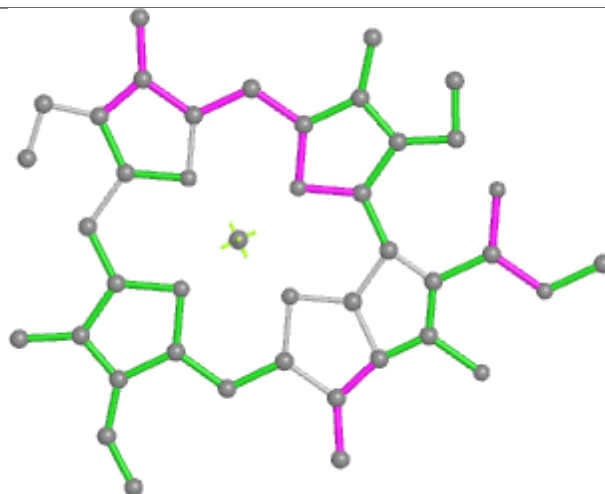
Ligand CLA A 813



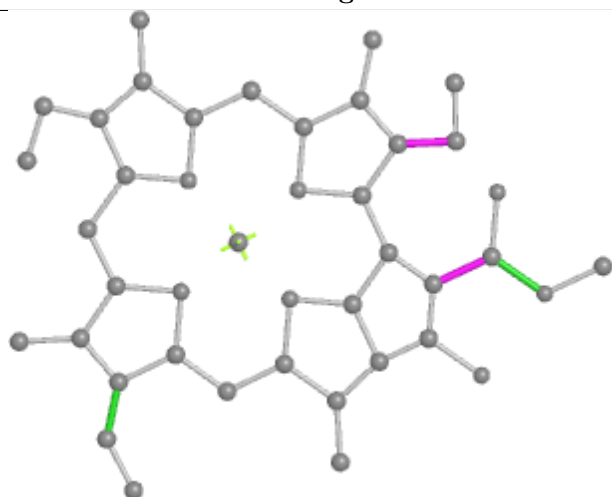
Ligand CLA A 814



Bond lengths



Bond angles

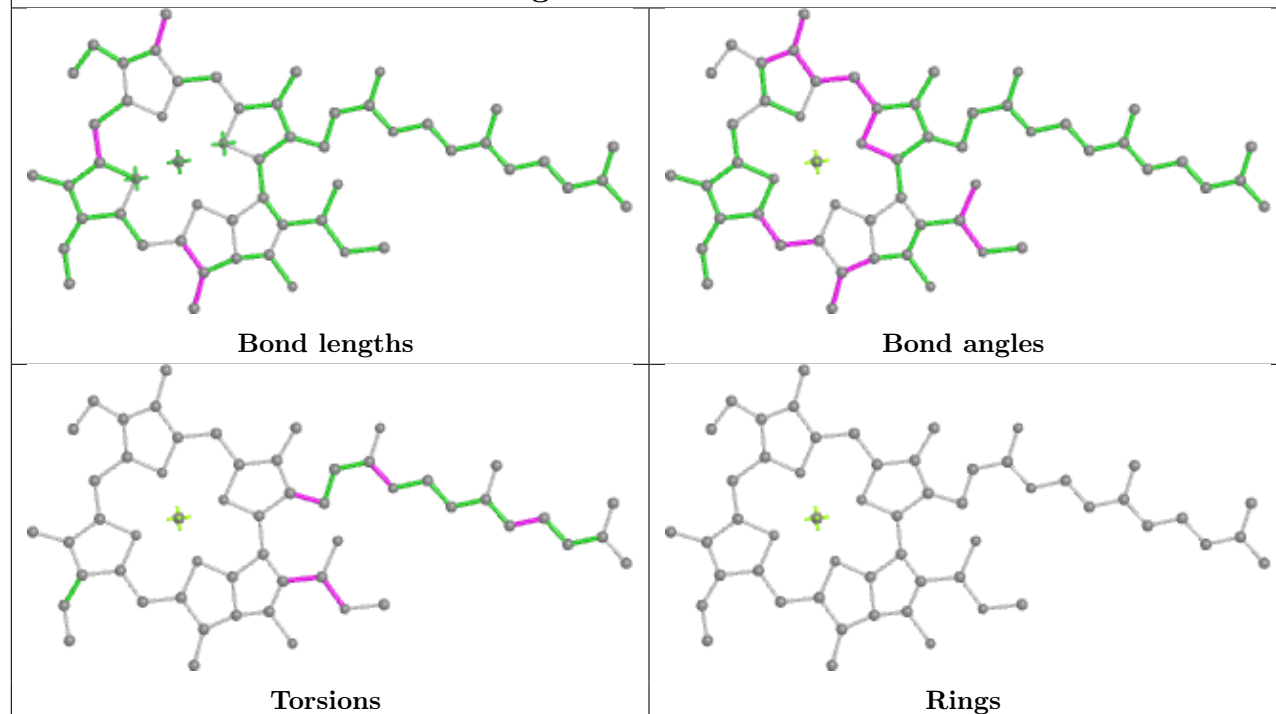


Torsions

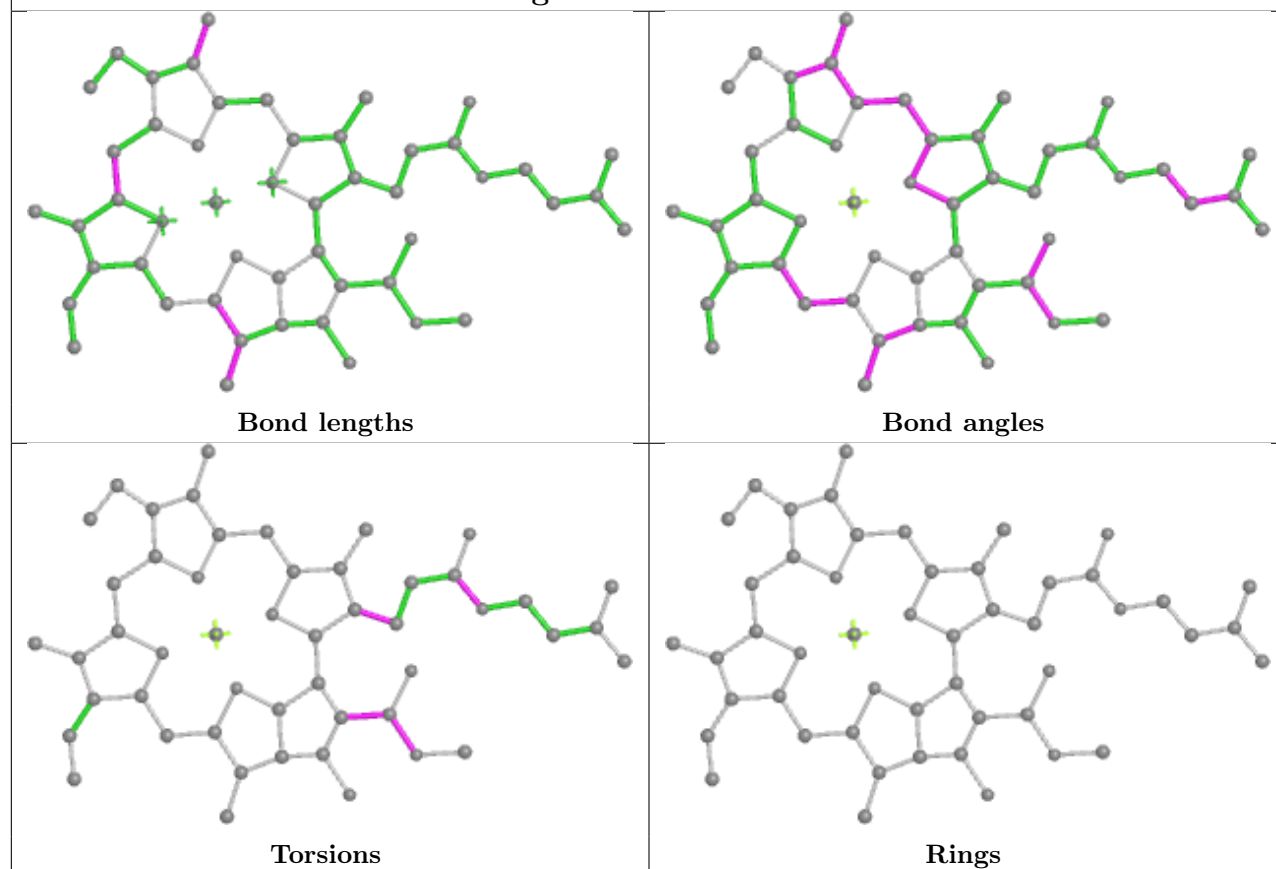


Rings

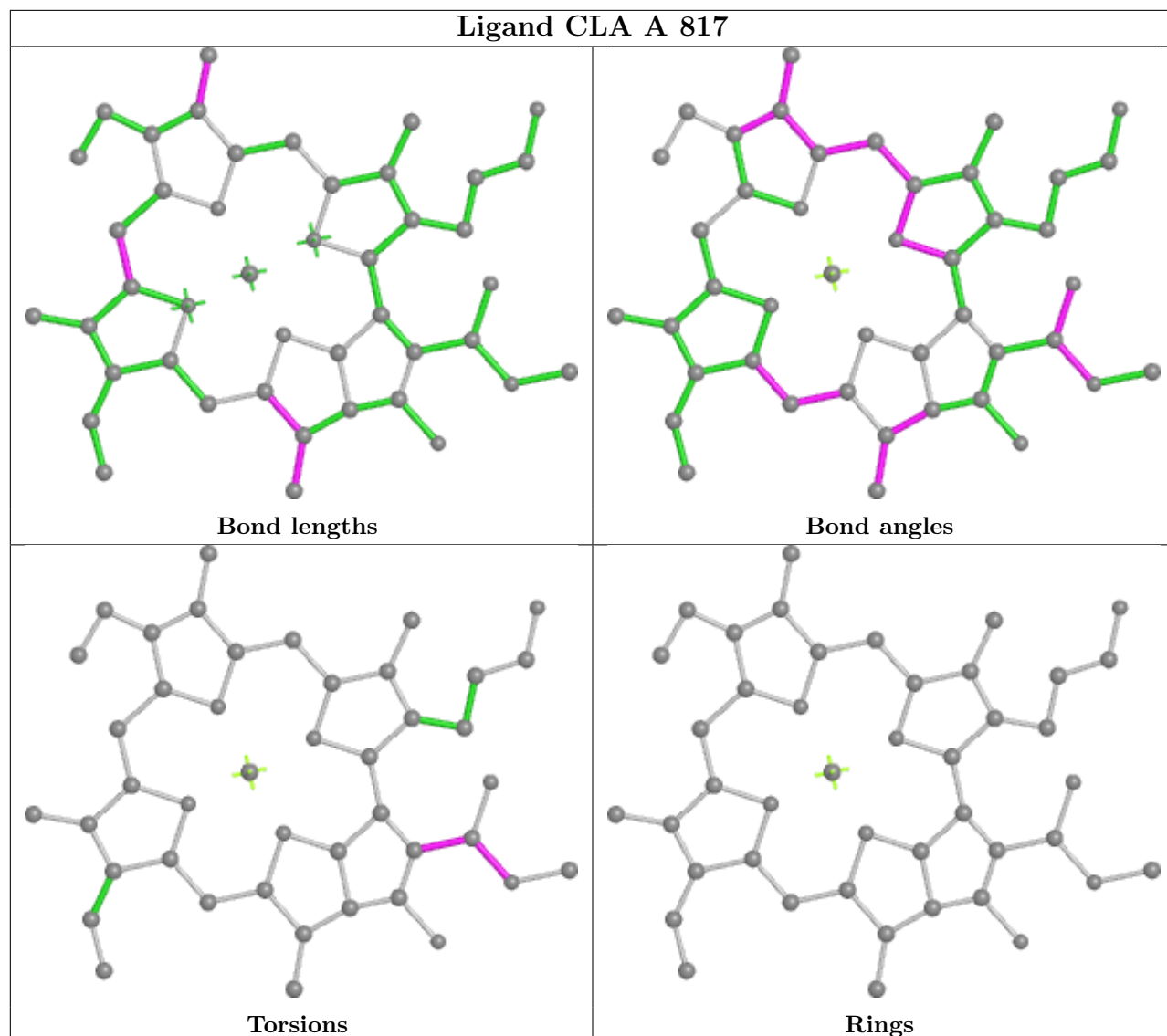
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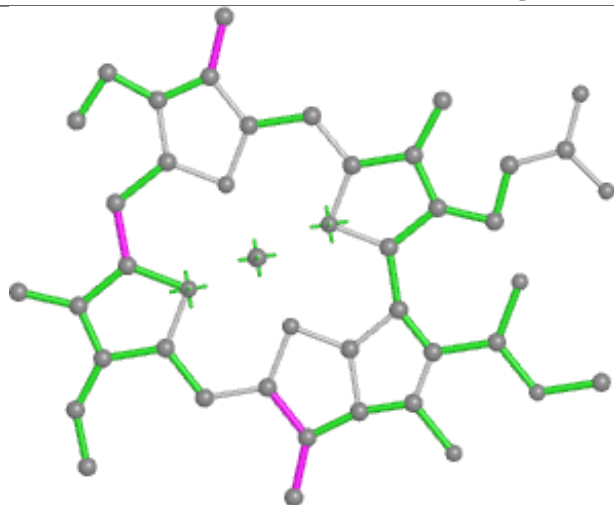
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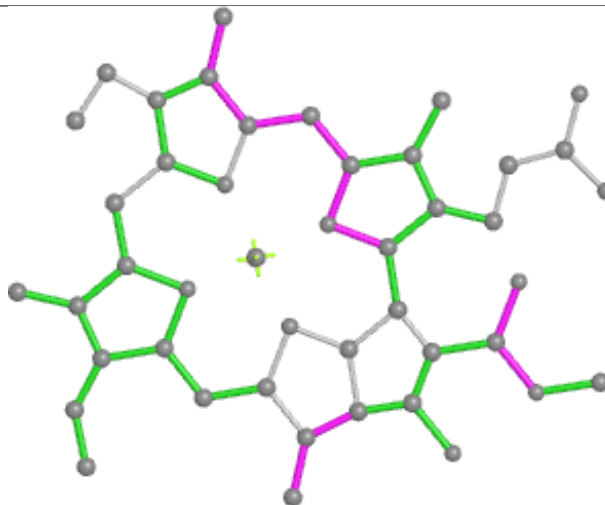
Ligand CLA A 817



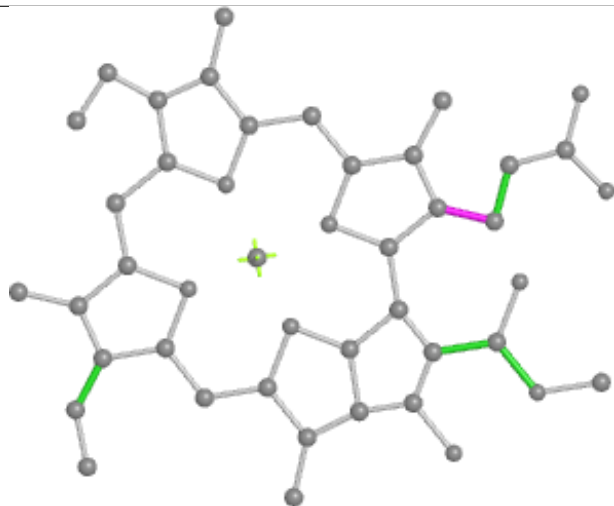
Ligand CLA A 818



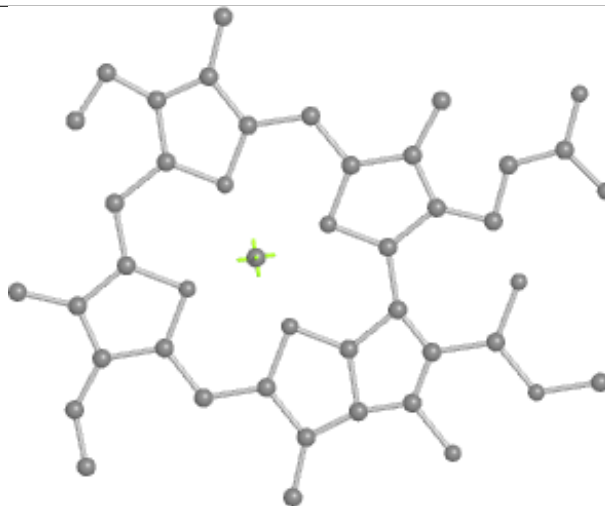
Bond lengths



Bond angles

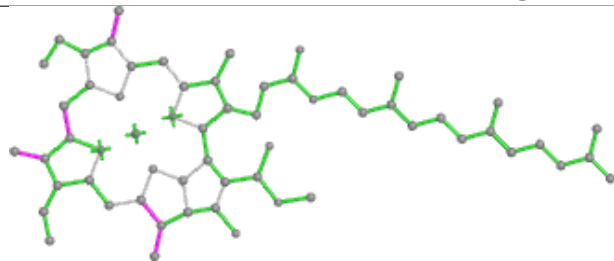


Torsions

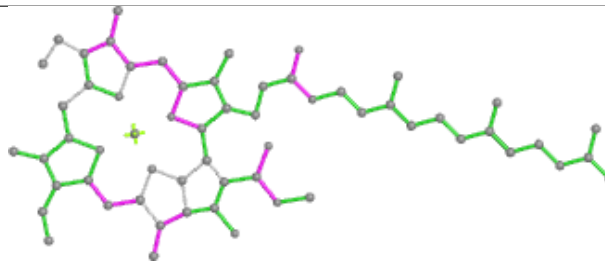


Rings

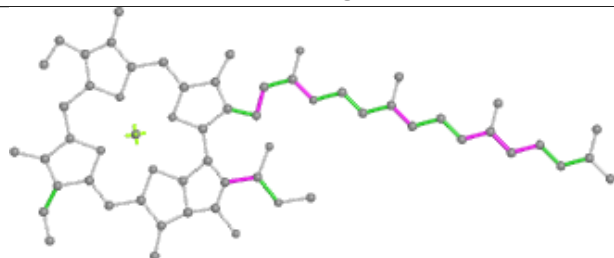
Ligand CLA A 819



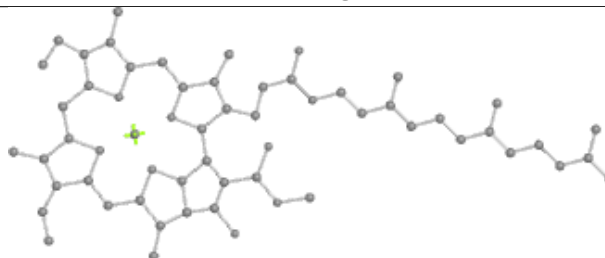
Bond lengths



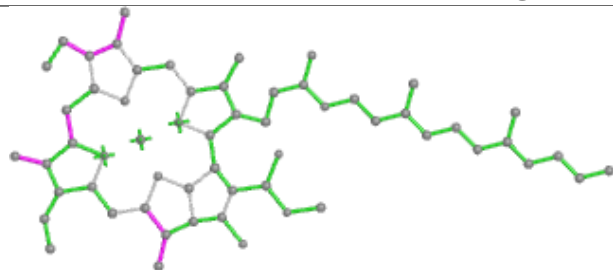
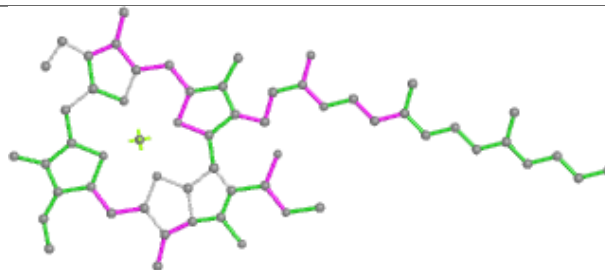
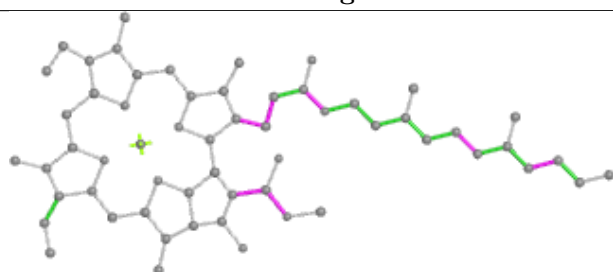
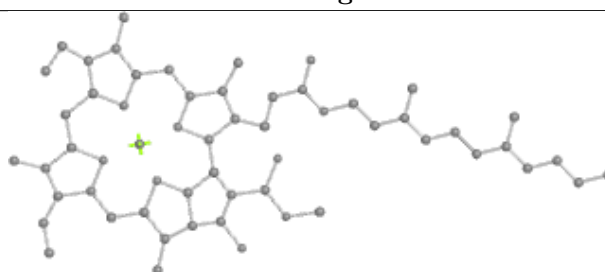
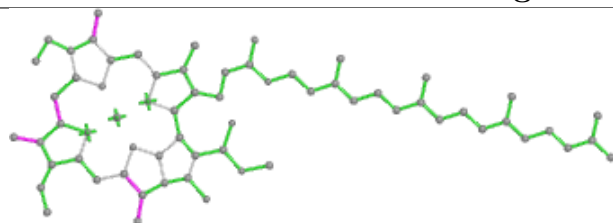
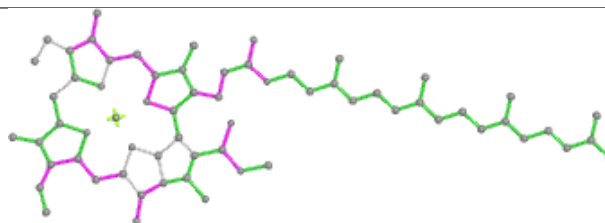
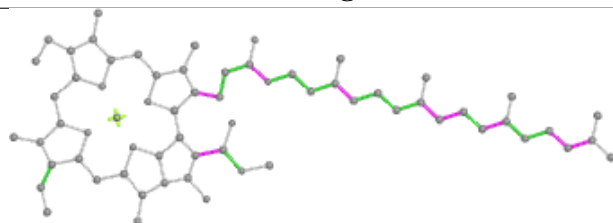
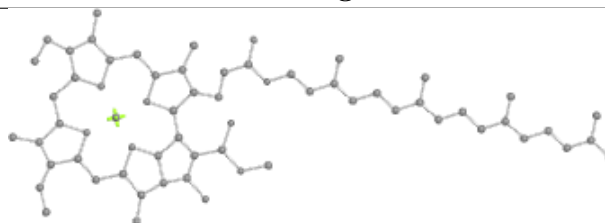
Bond angles



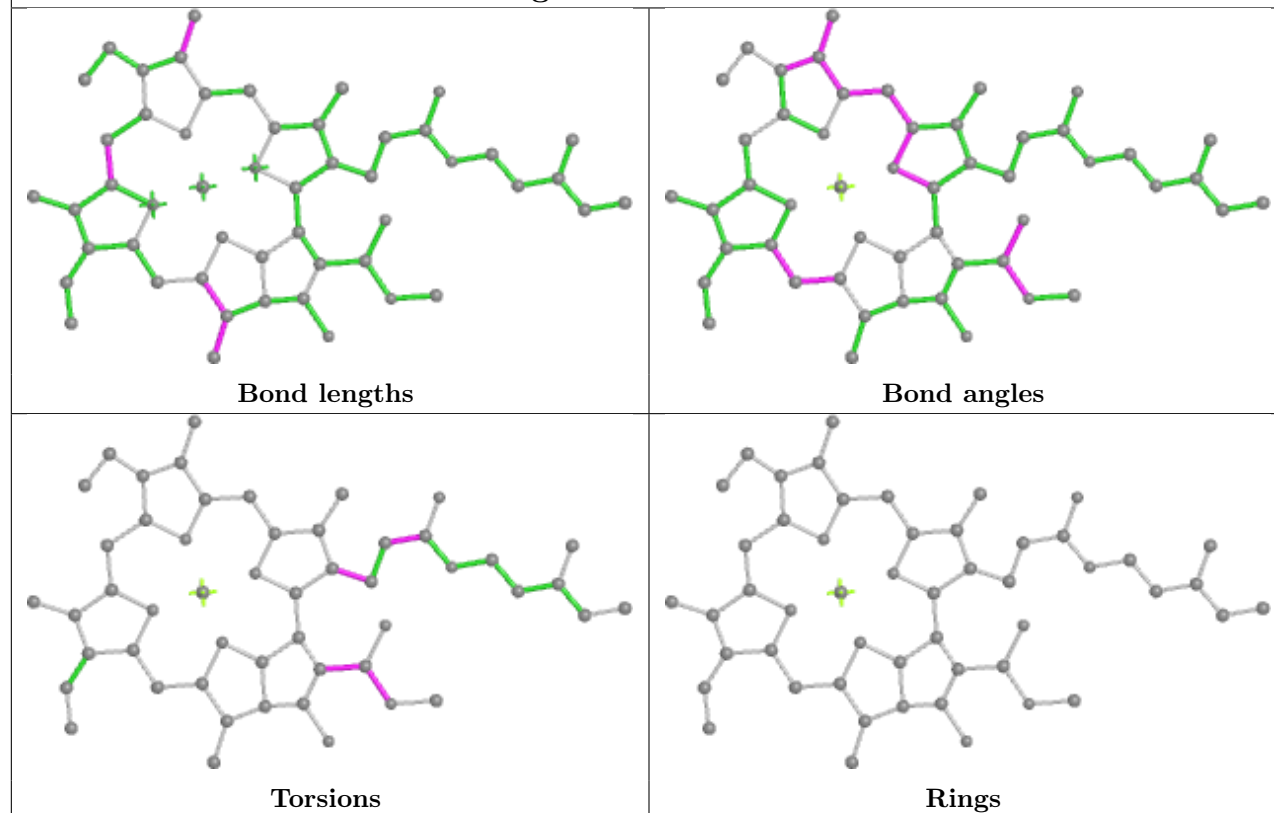
Torsions



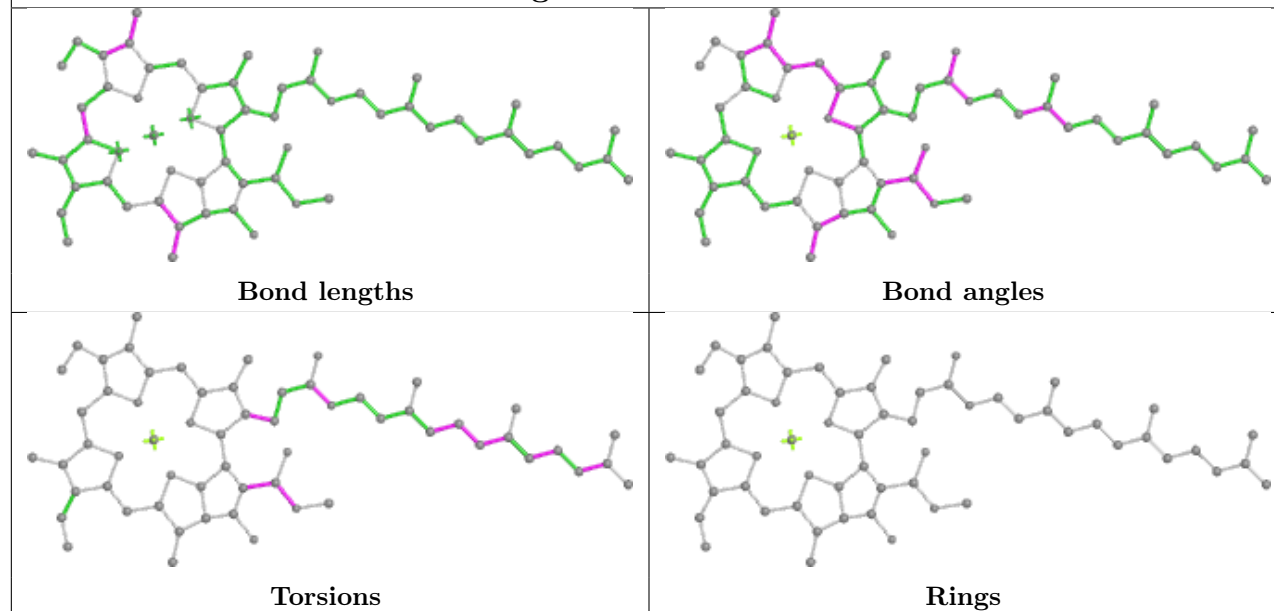
Rings

Ligand CLA A 820**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 821****Bond lengths****Bond angles****Torsions****Rings**

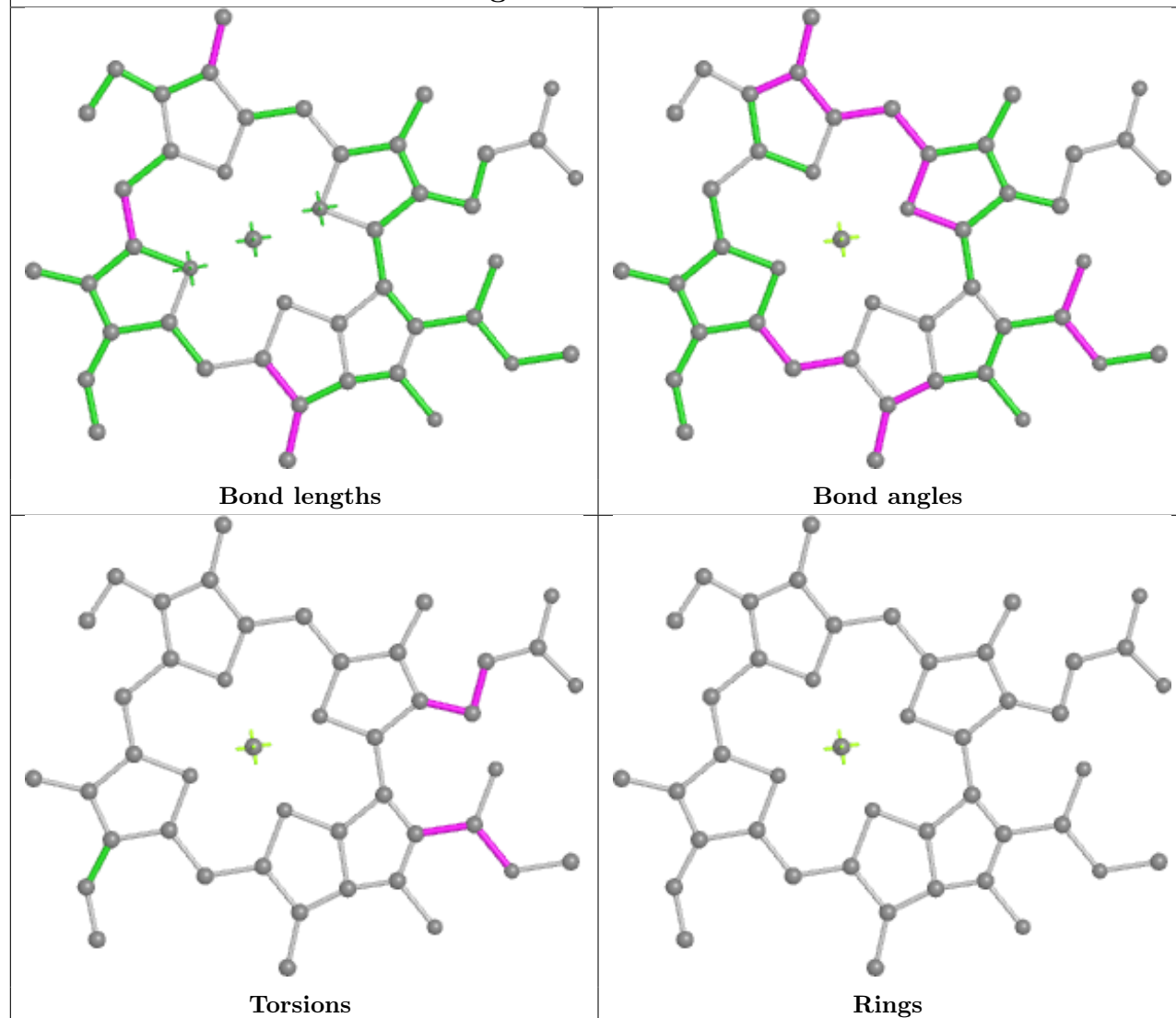
Ligand CLA A 822

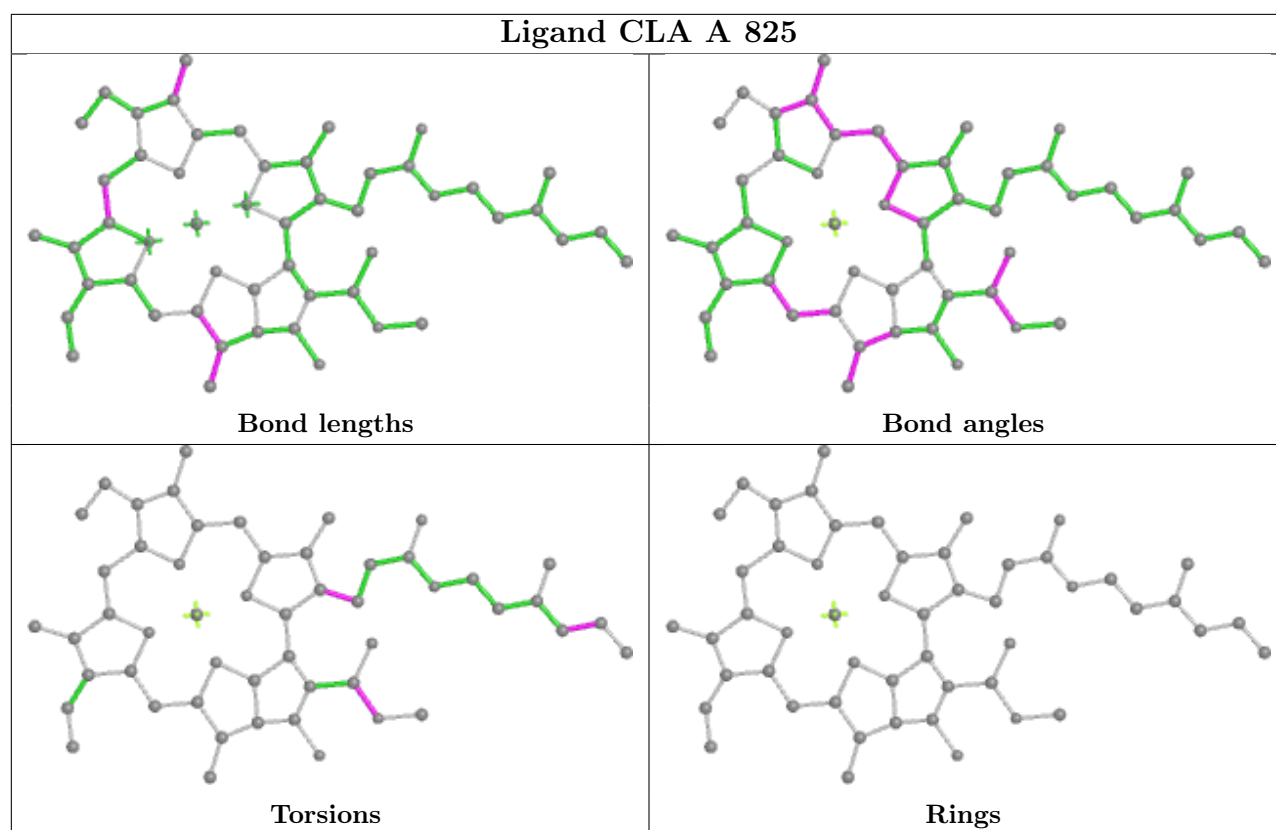


Ligand CLA A 823

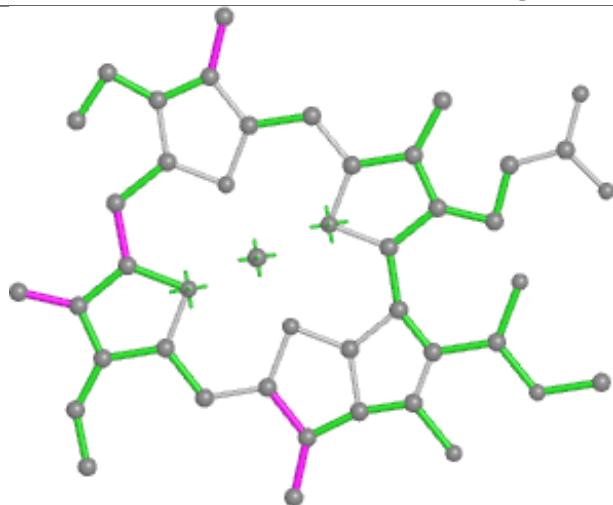


Ligand CLA A 824

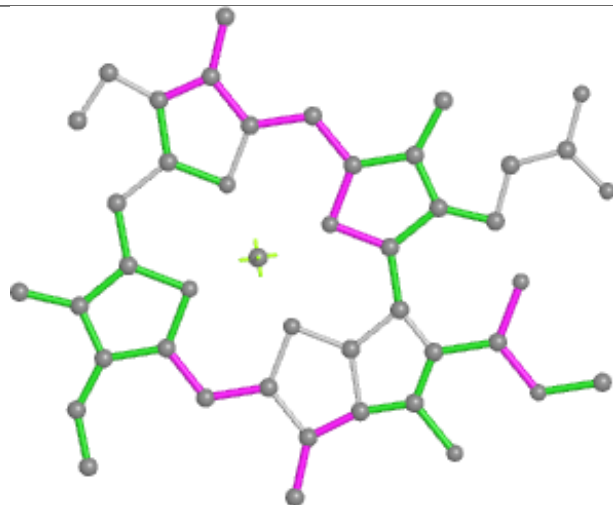




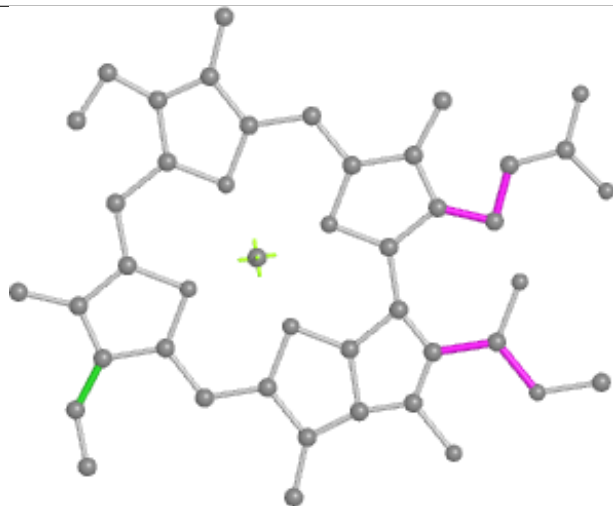
Ligand CLA A 826



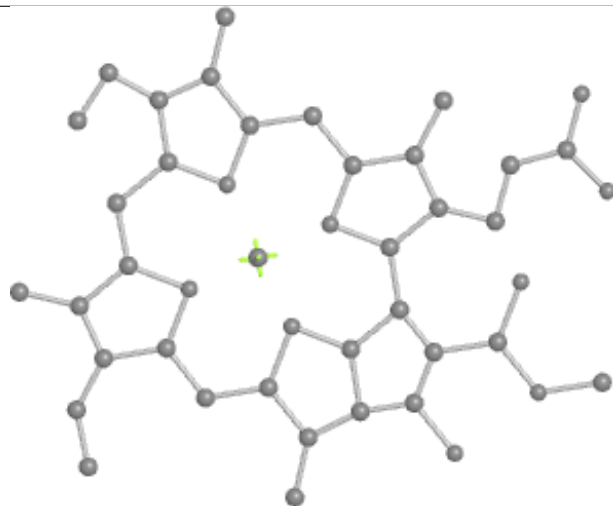
Bond lengths



Bond angles

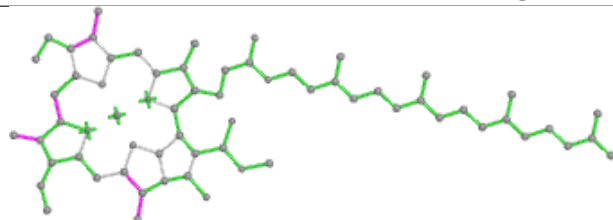


Torsions

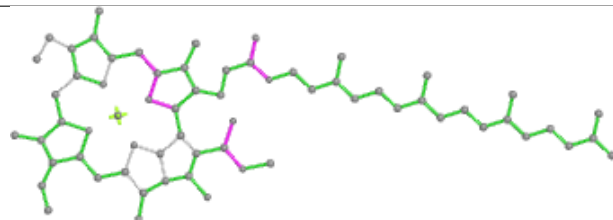


Rings

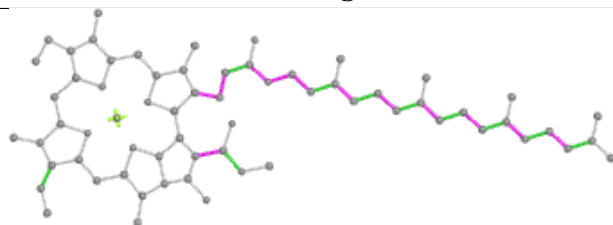
Ligand CLA A 827



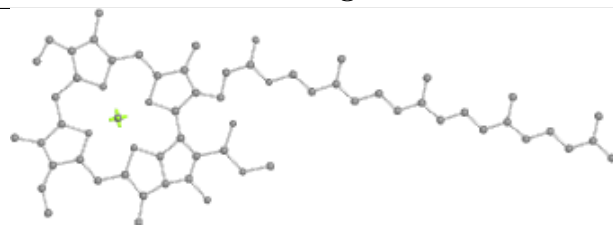
Bond lengths



Bond angles

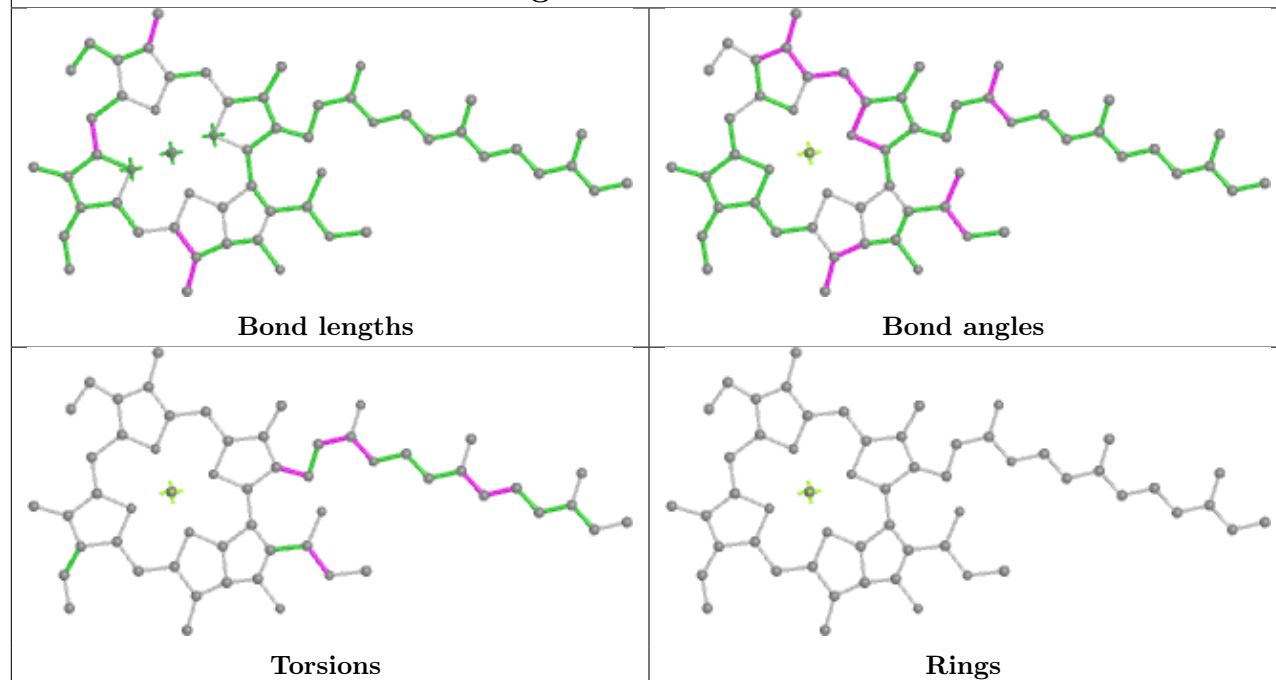


Torsions

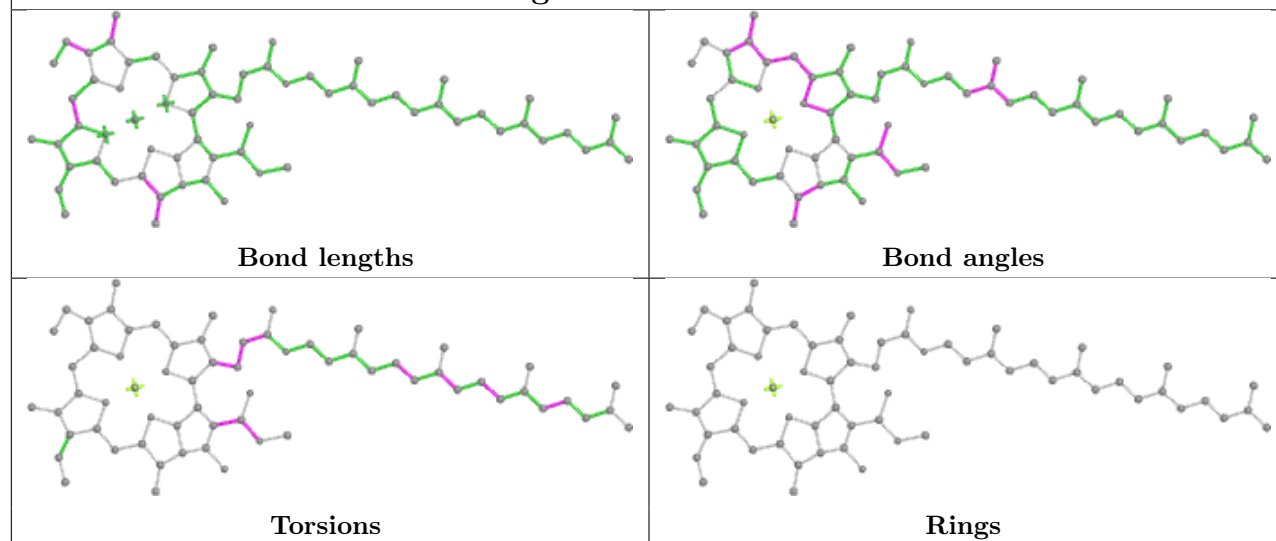


Rings

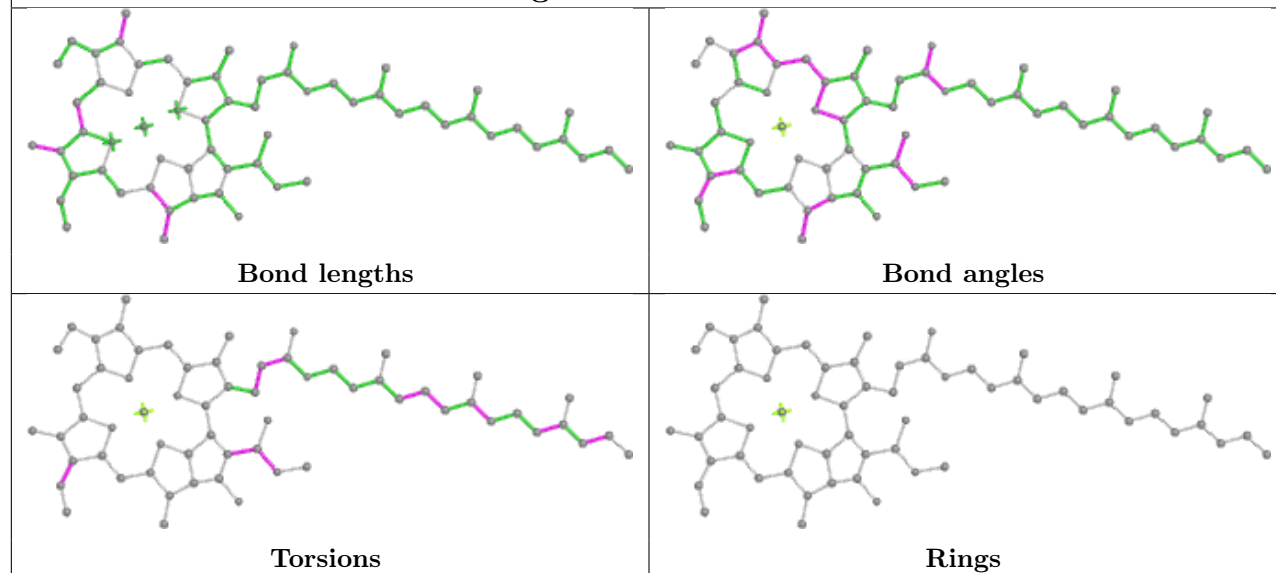
Ligand CLA A 828



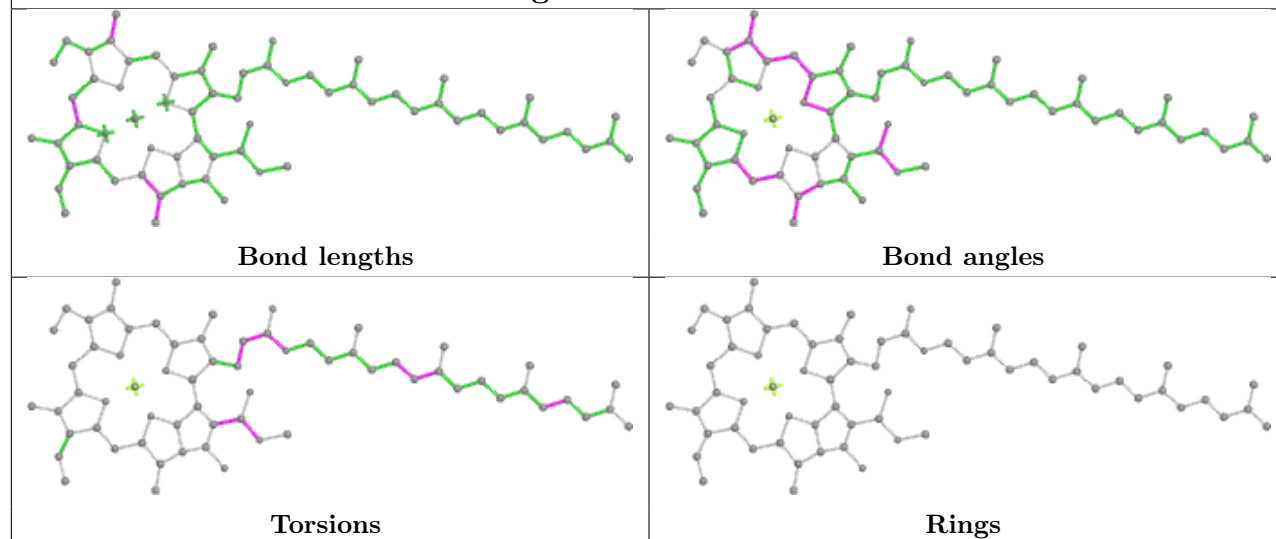
Ligand CLA A 829



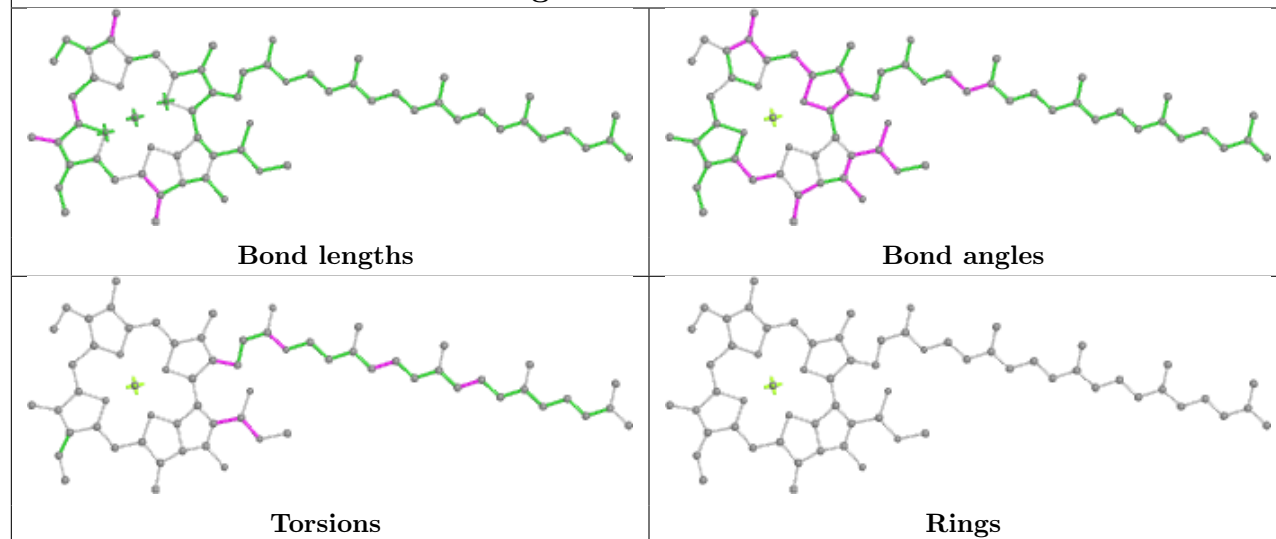
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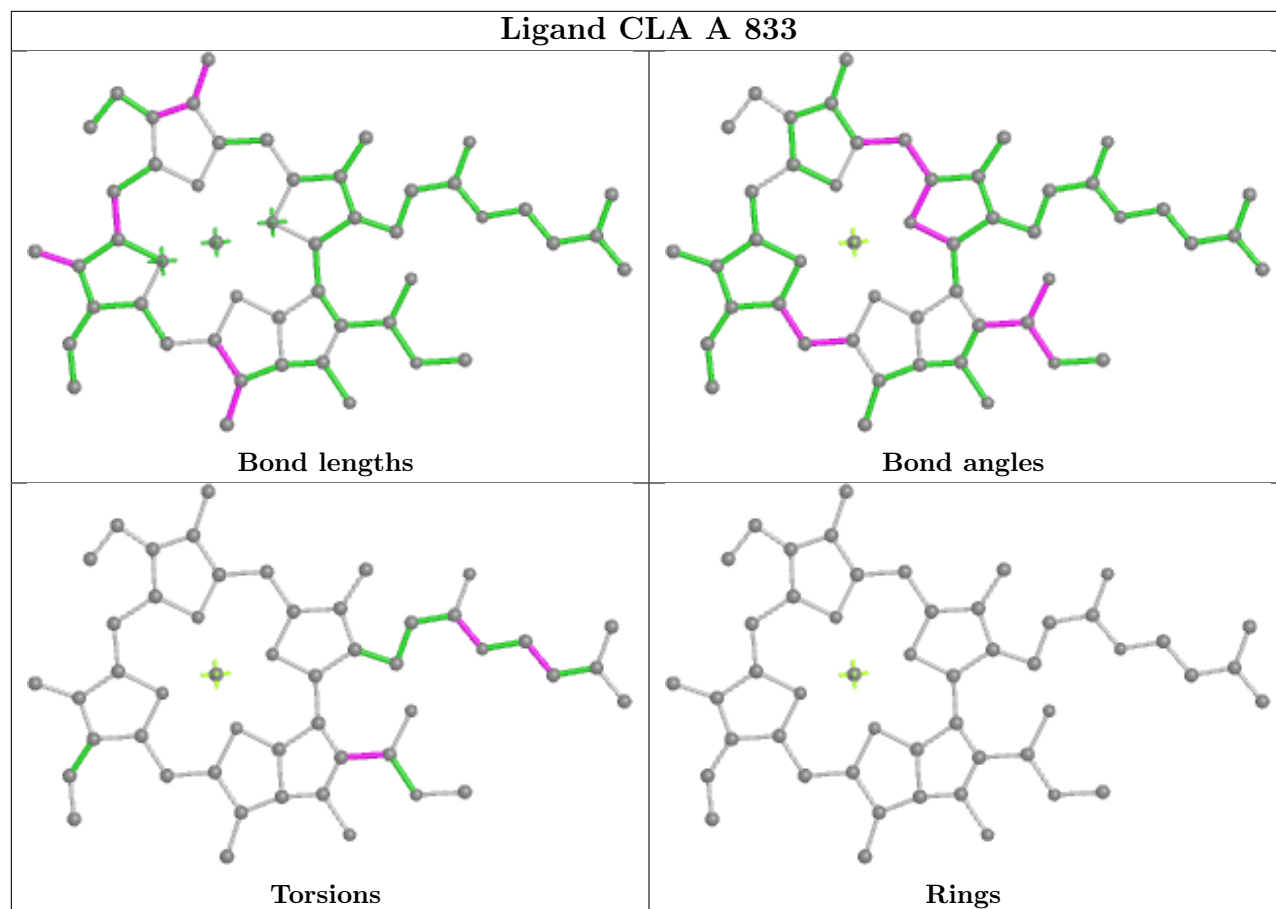
Ligand CLA A 831



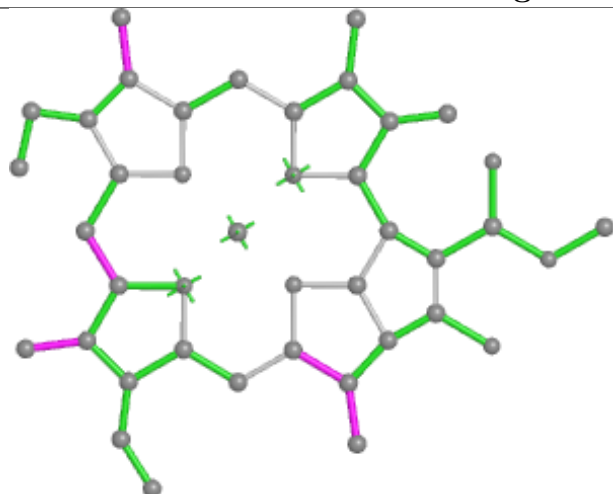
Ligand CLA A 832



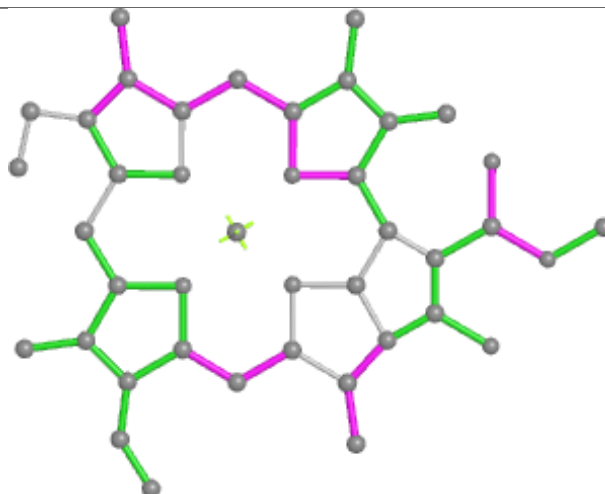
Ligand CLA A 833



Ligand CLA A 834



Bond lengths



Bond angles

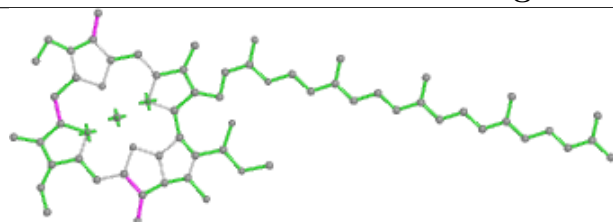


Torsions

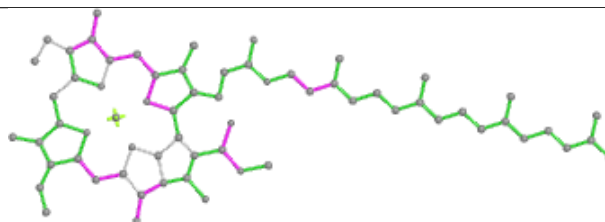


Rings

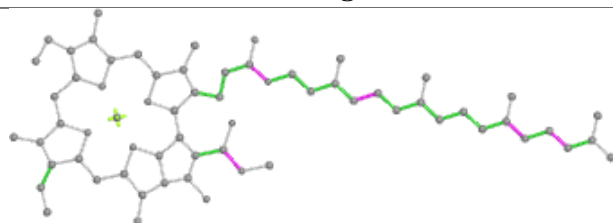
Ligand CLA A 835



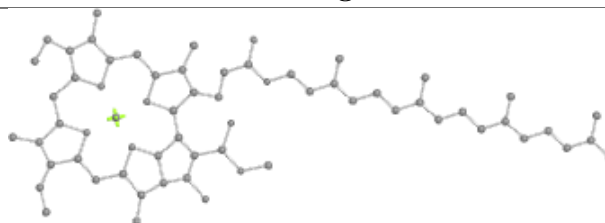
Bond lengths



Bond angles

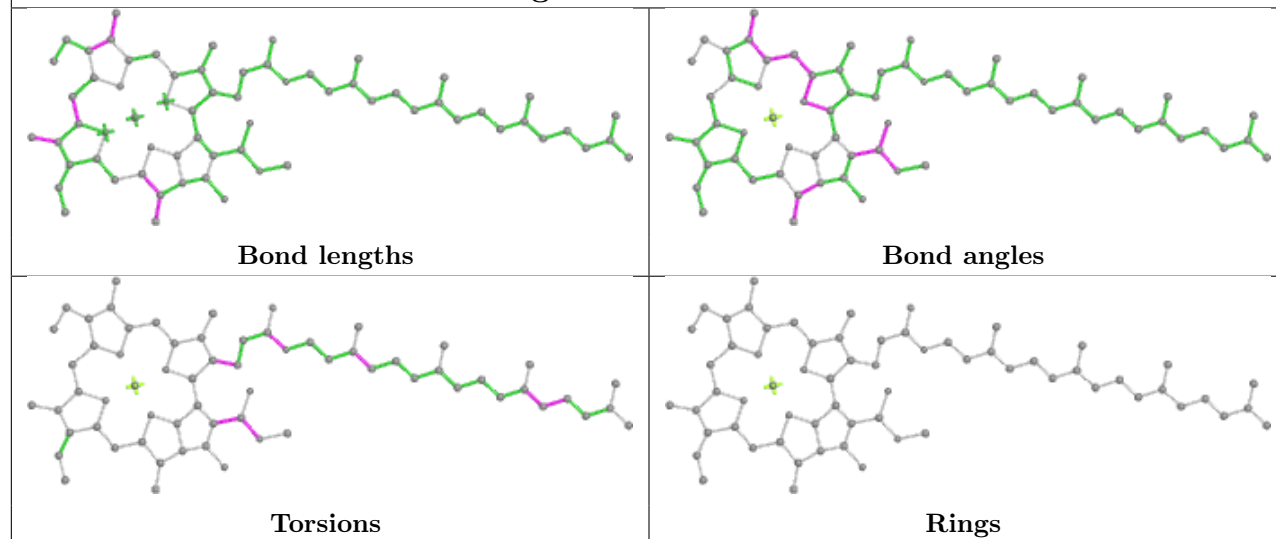


Torsions

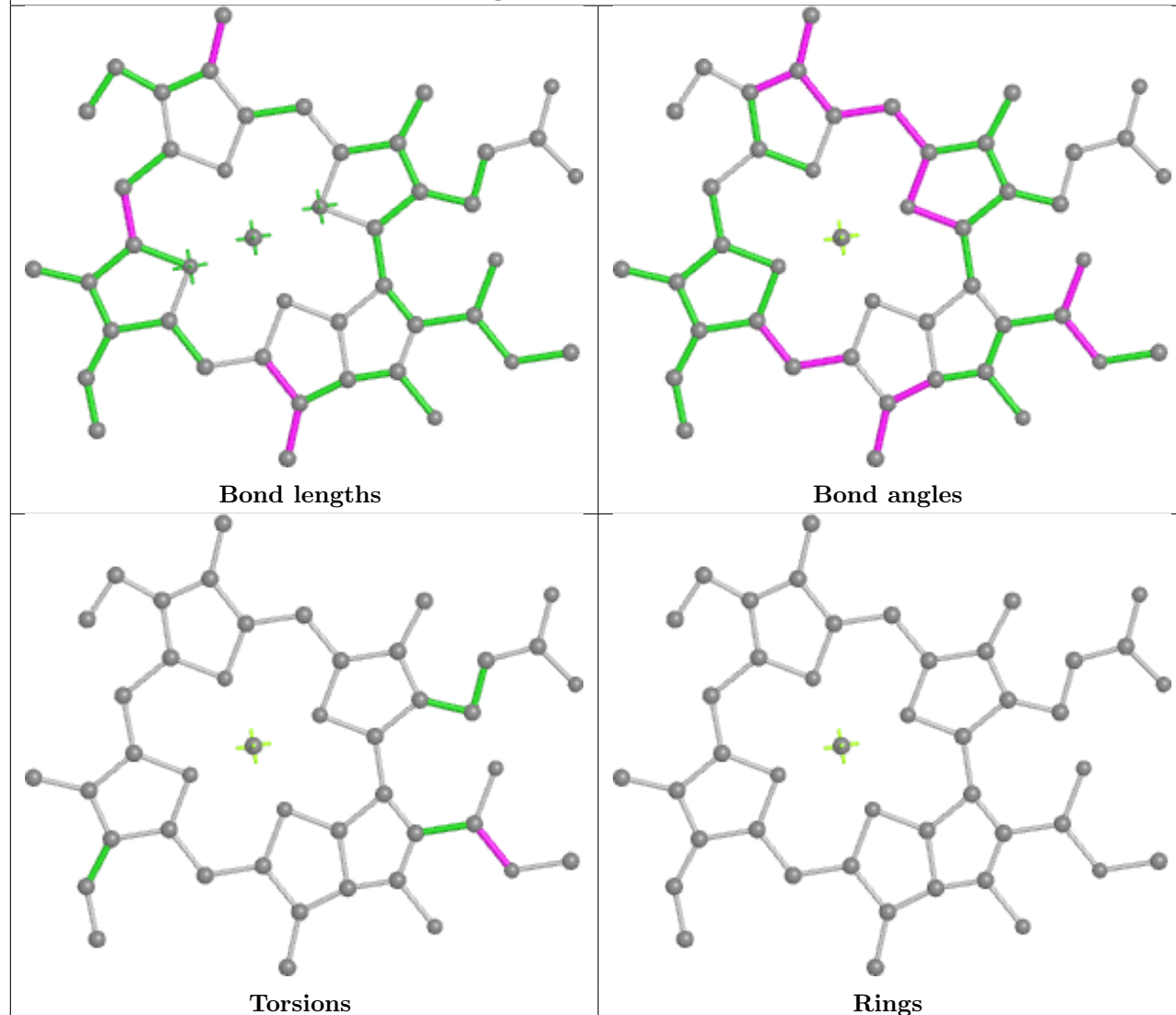


Rings

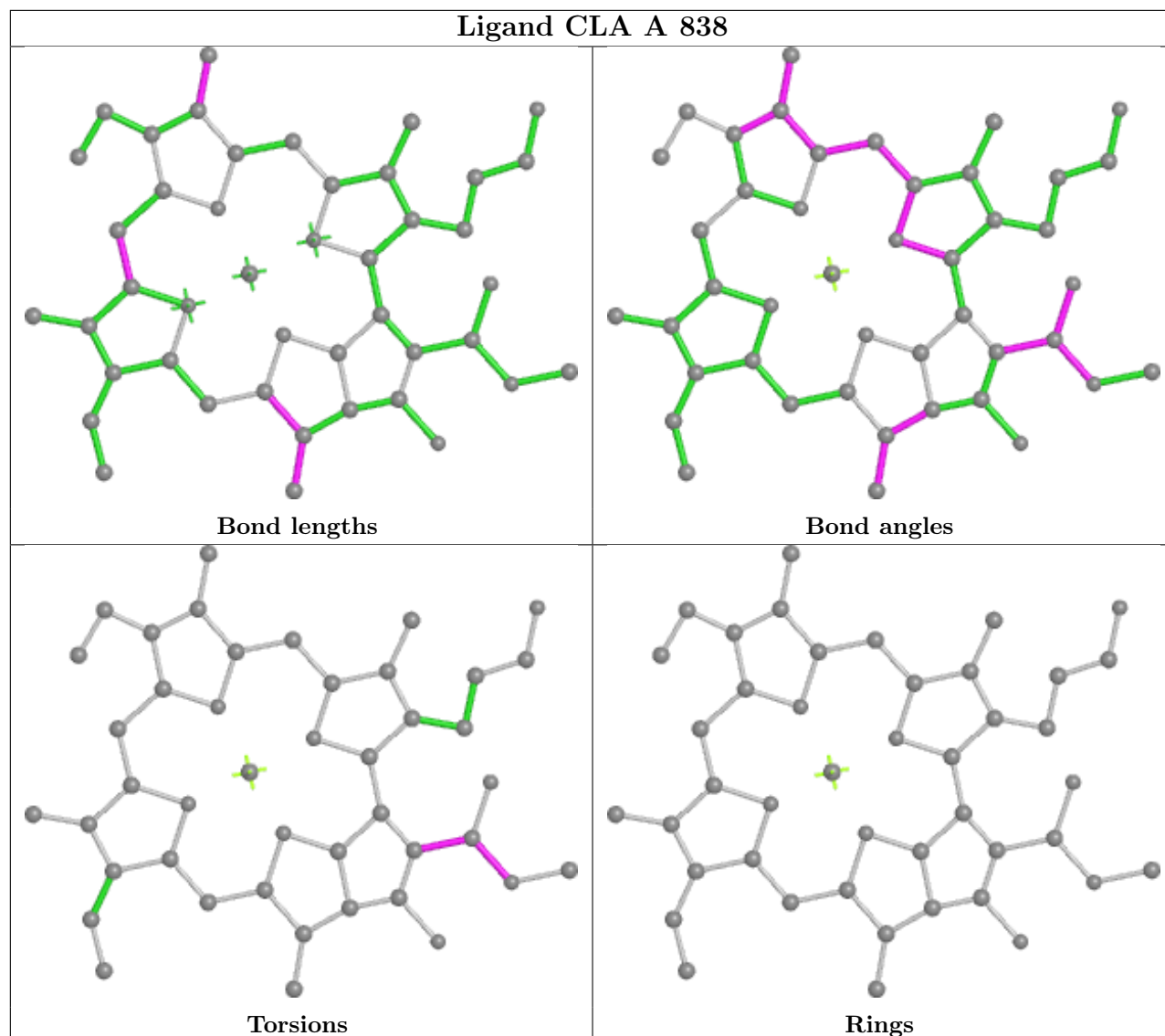
Ligand CLA A 836



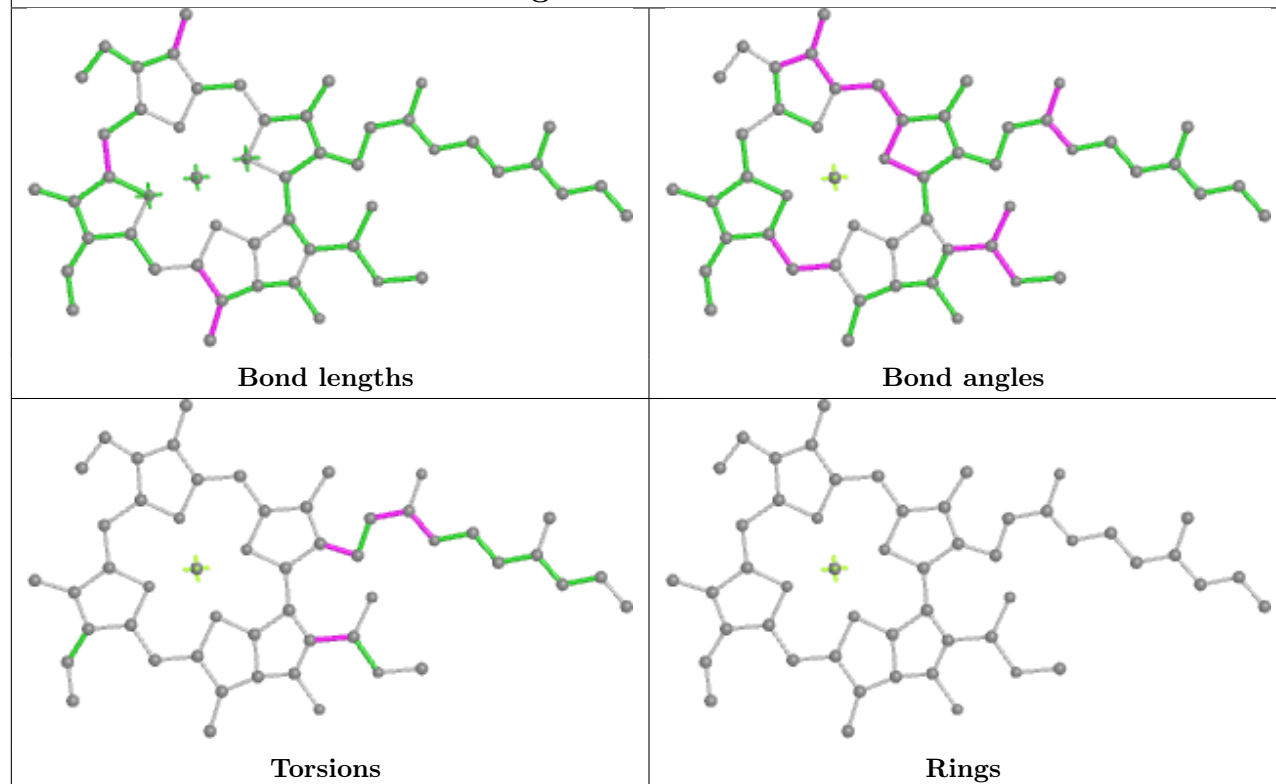
Ligand CLA A 837



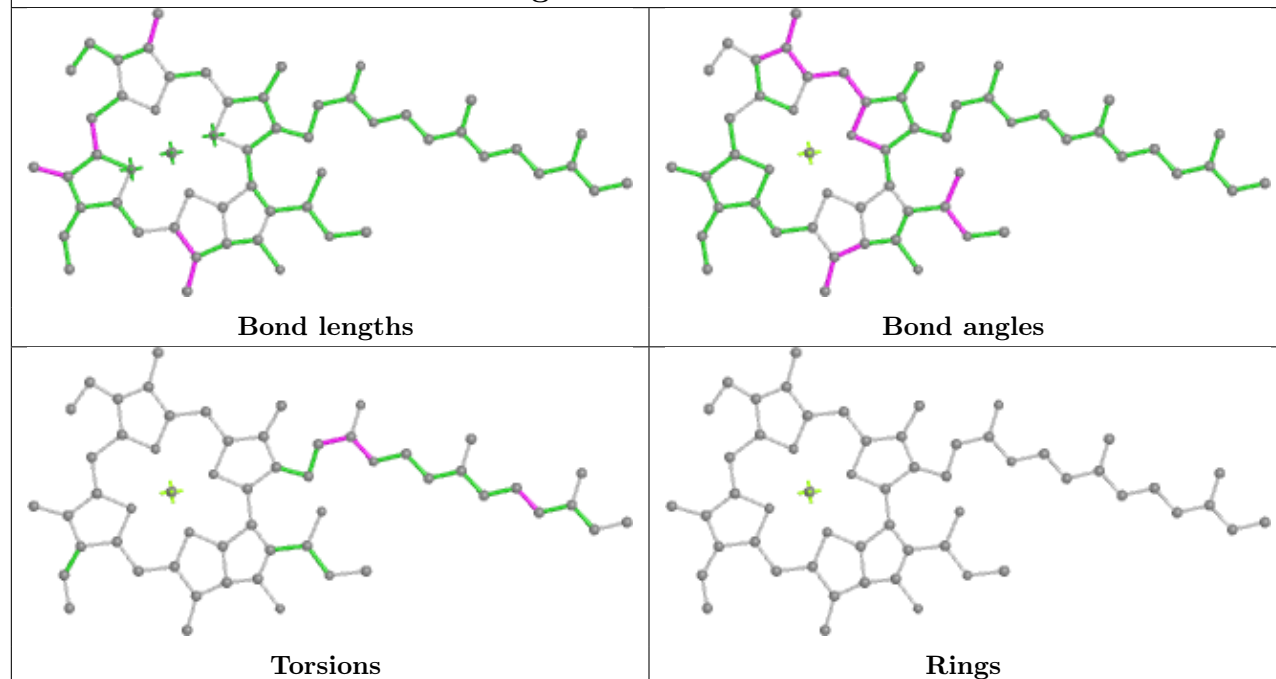
Ligand CLA A 838



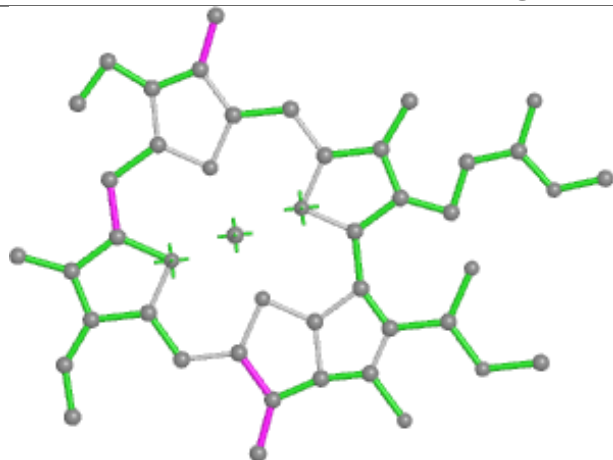
Ligand CLA A 839



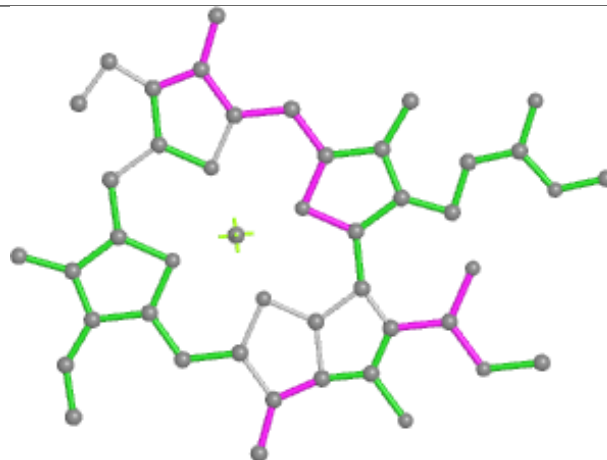
Ligand CLA A 840



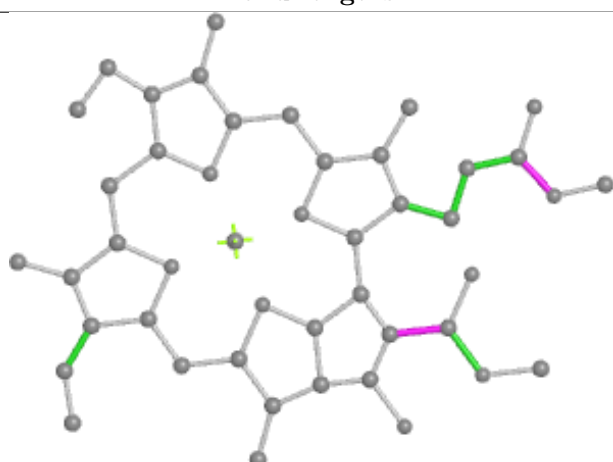
Ligand CLA A 841



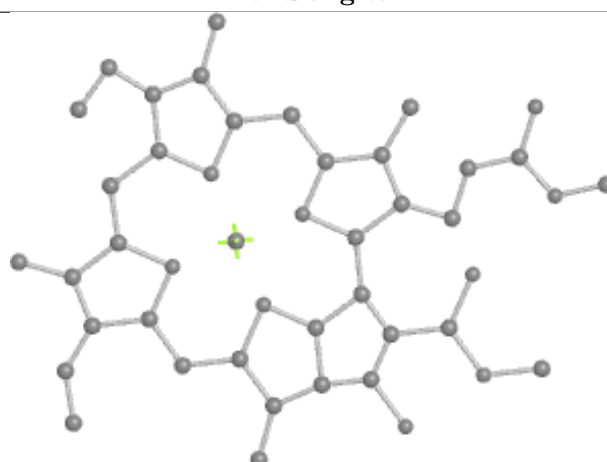
Bond lengths



Bond angles

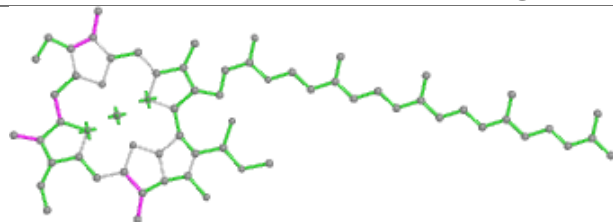


Torsions

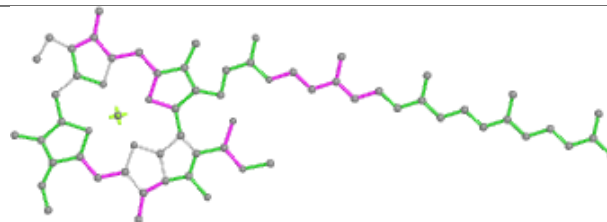


Rings

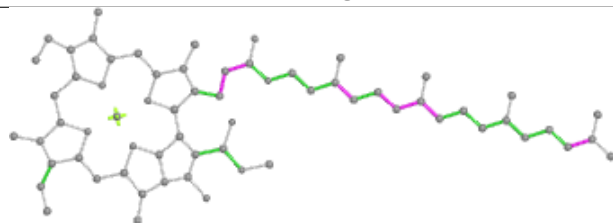
Ligand CLA A 842



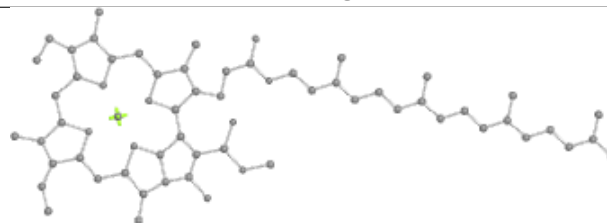
Bond lengths



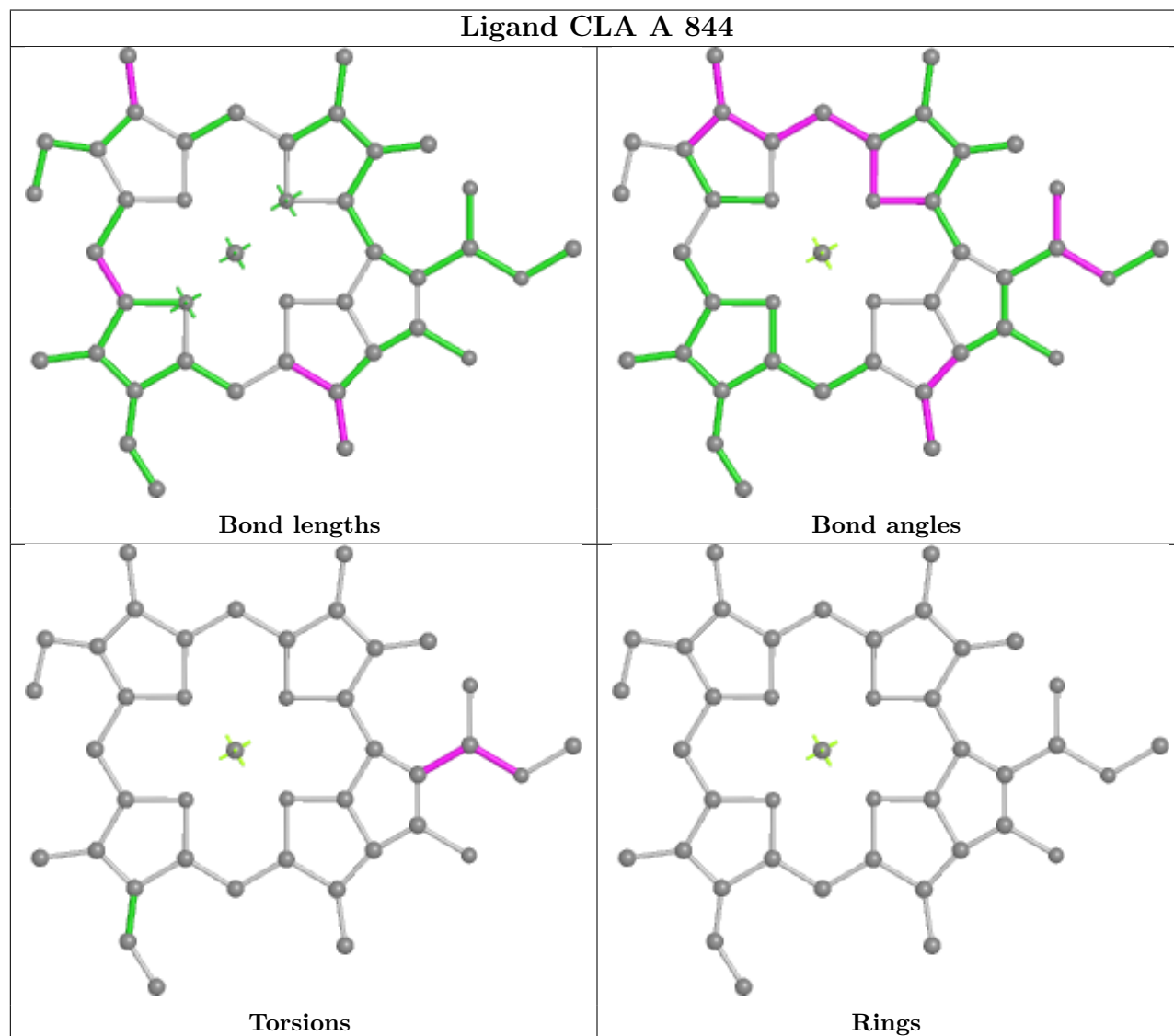
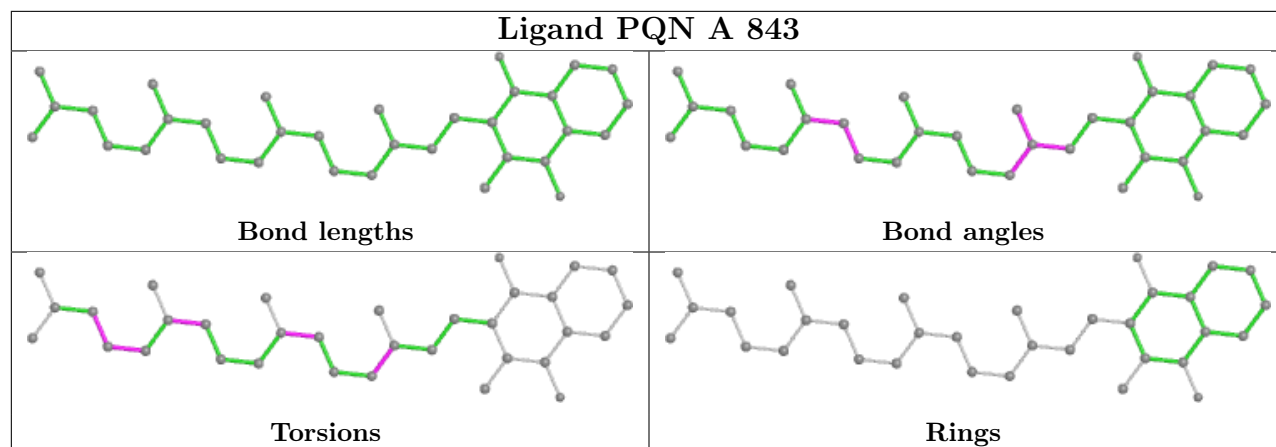
Bond angles

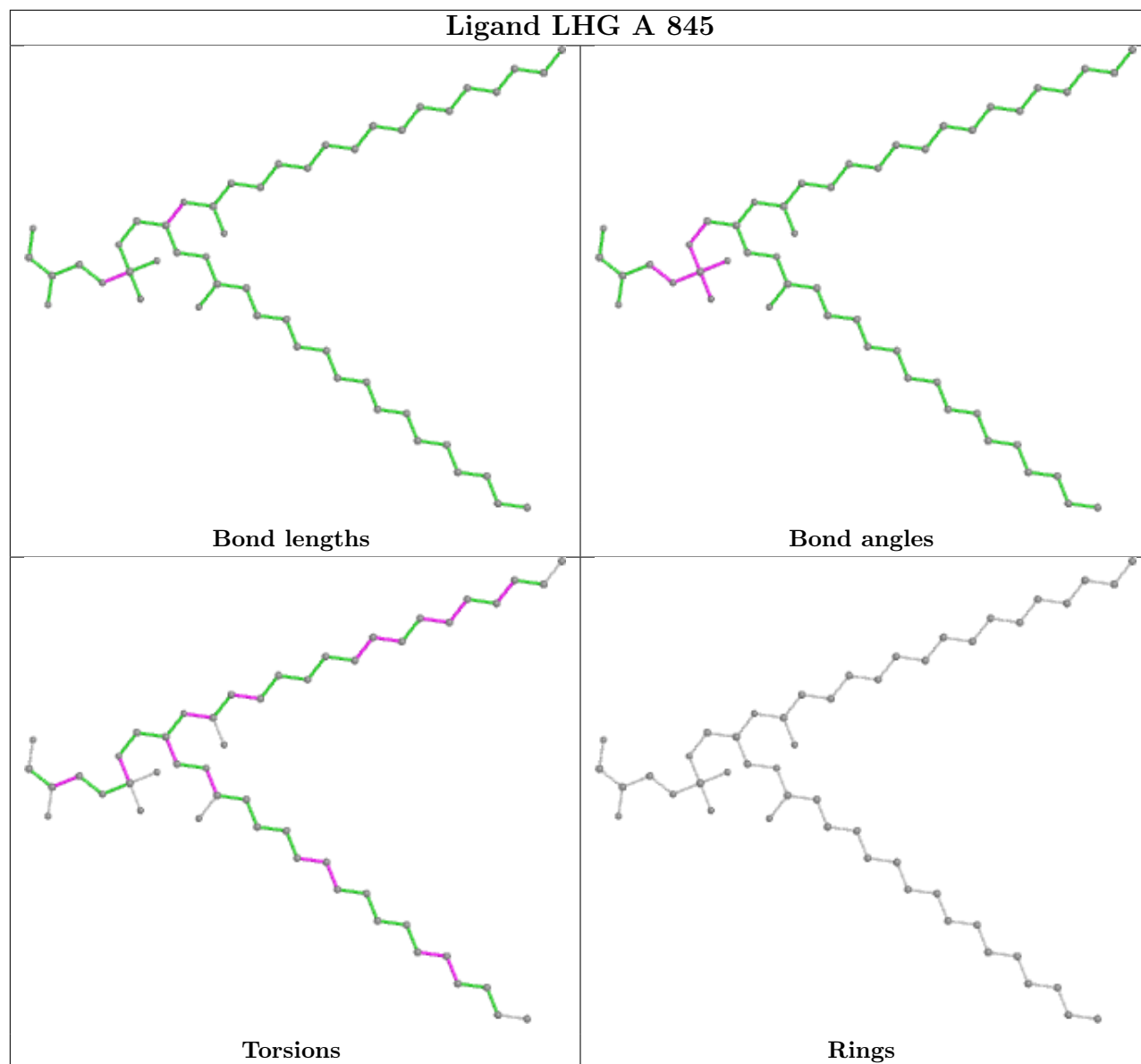


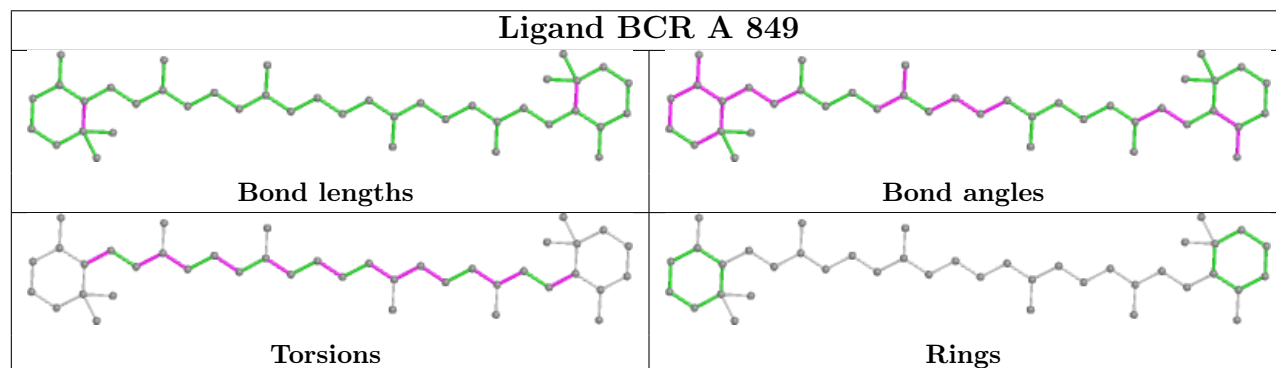
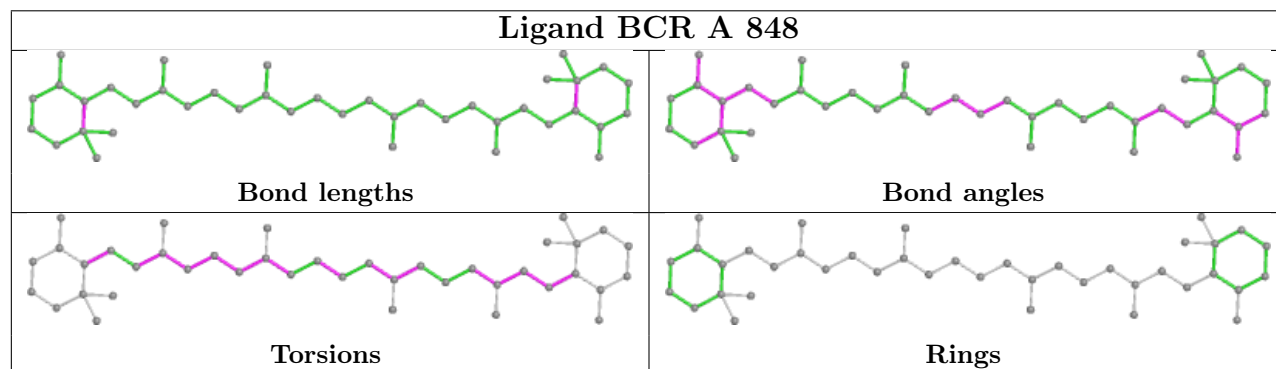
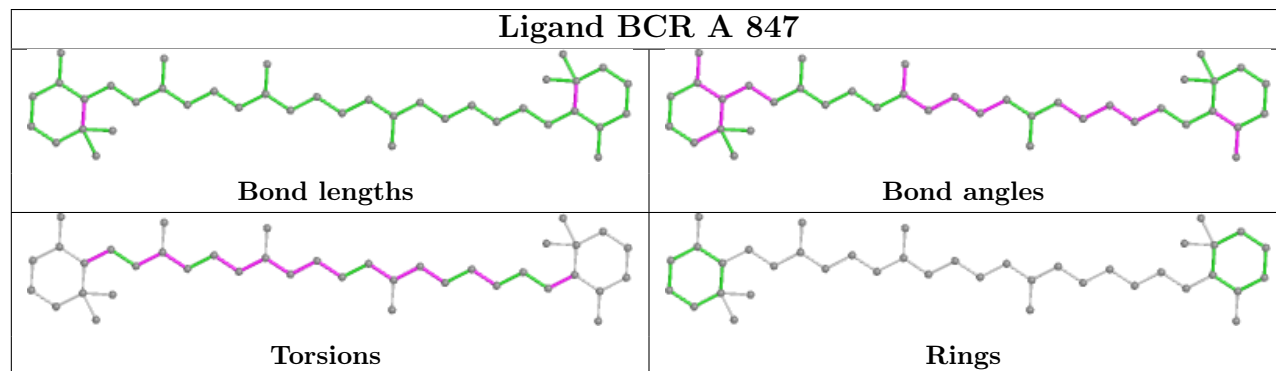
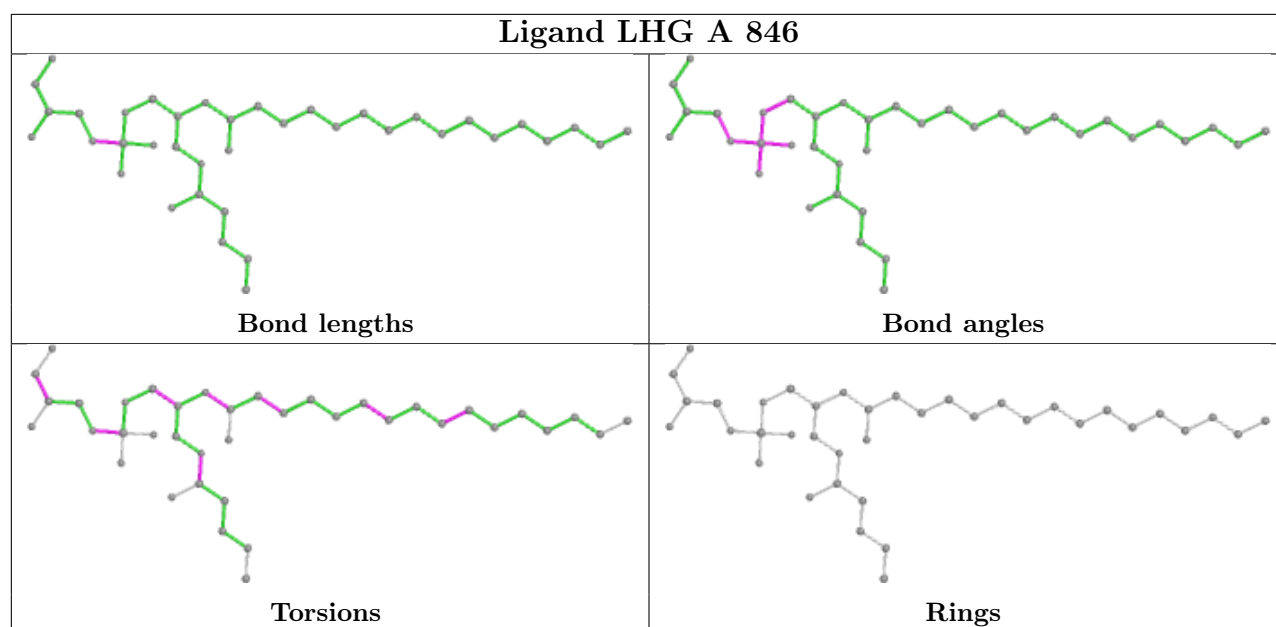
Torsions

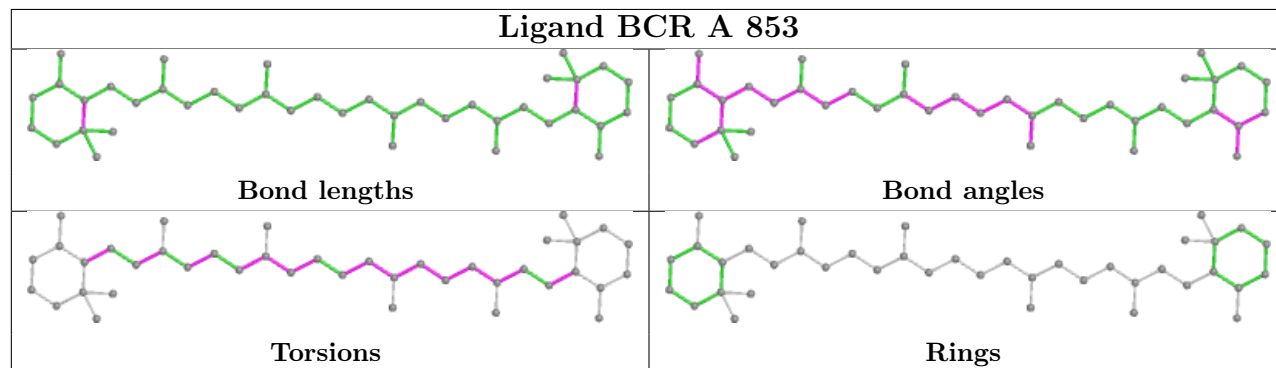
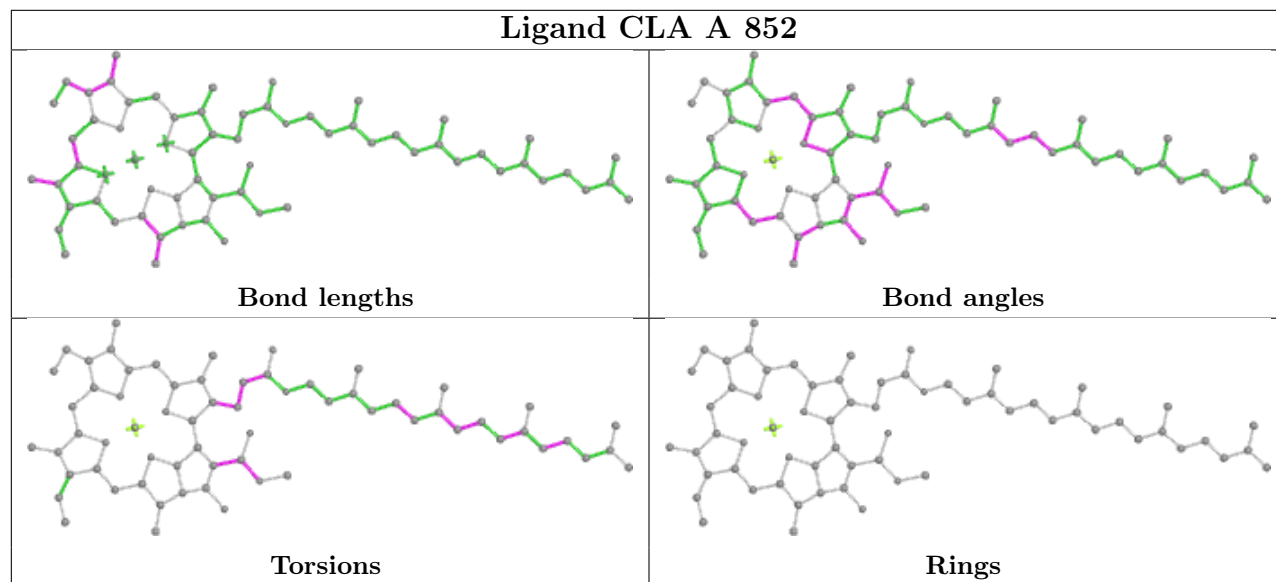
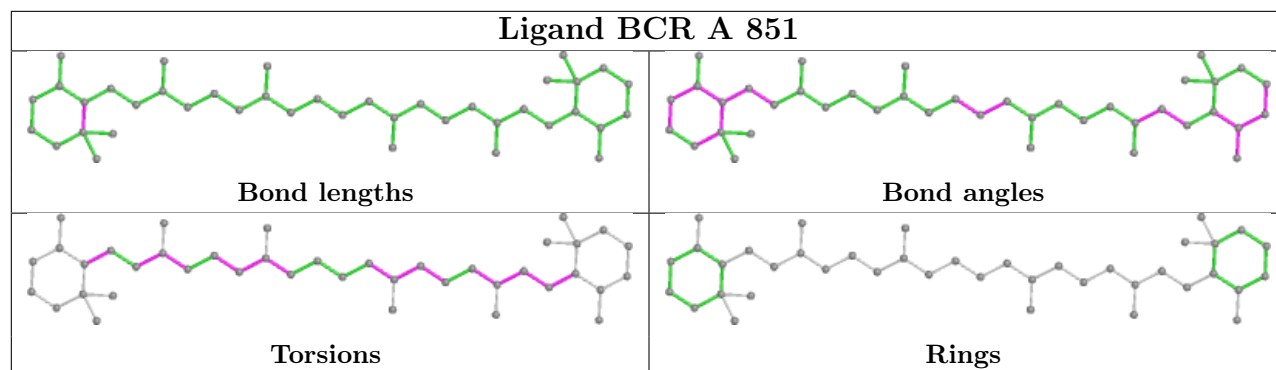
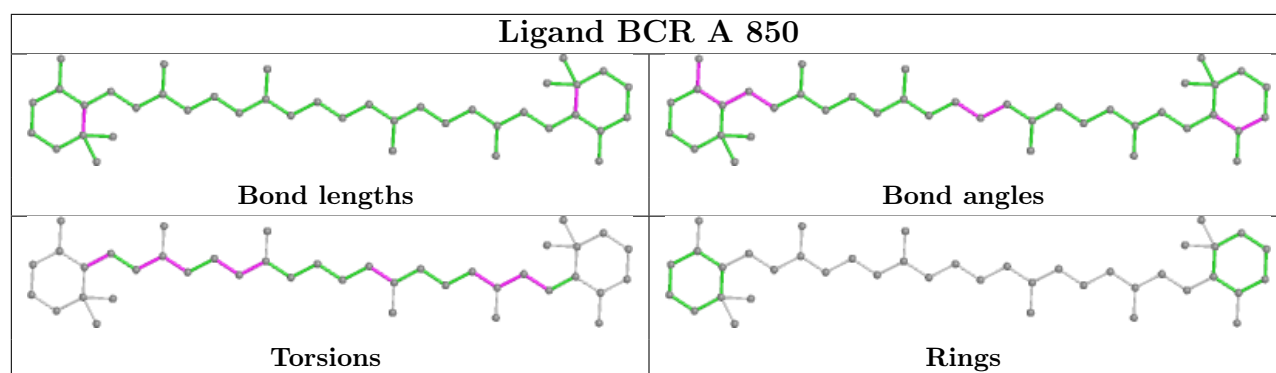


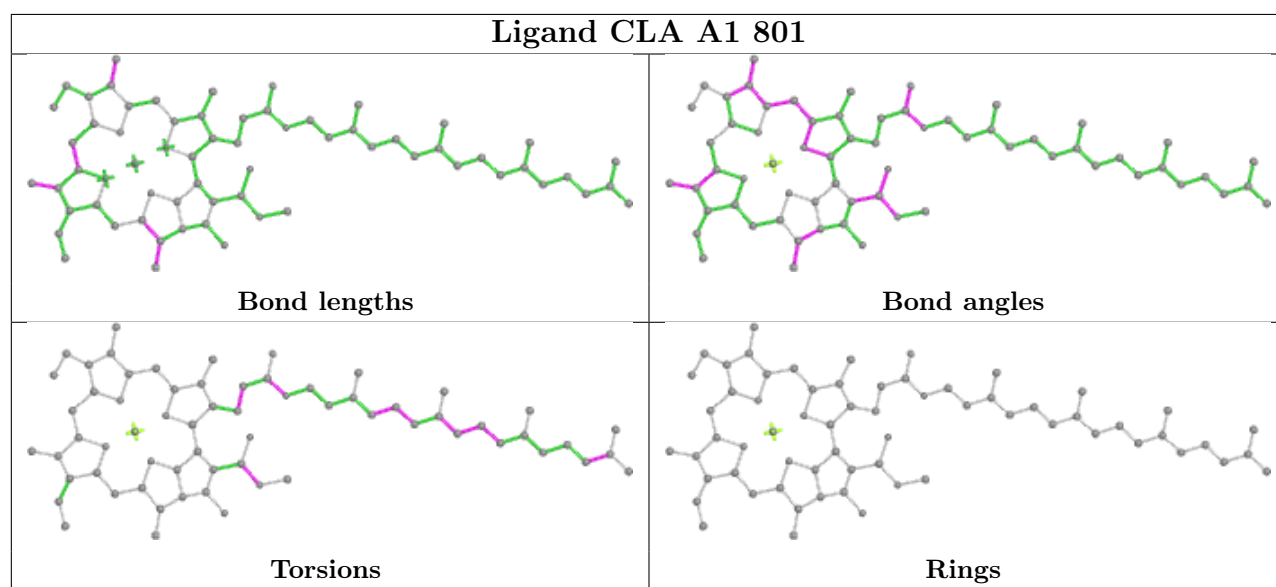
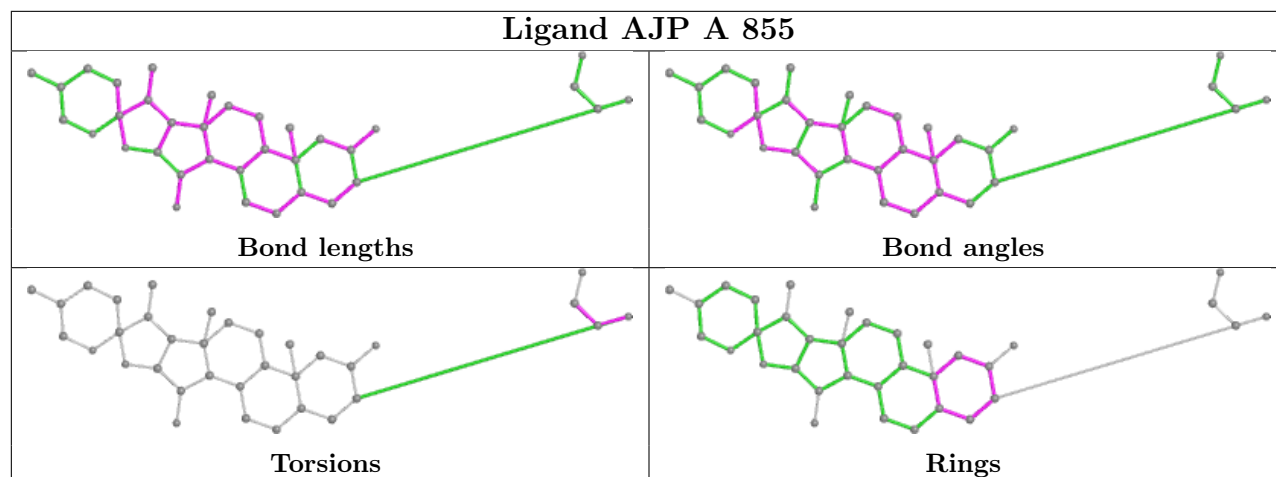
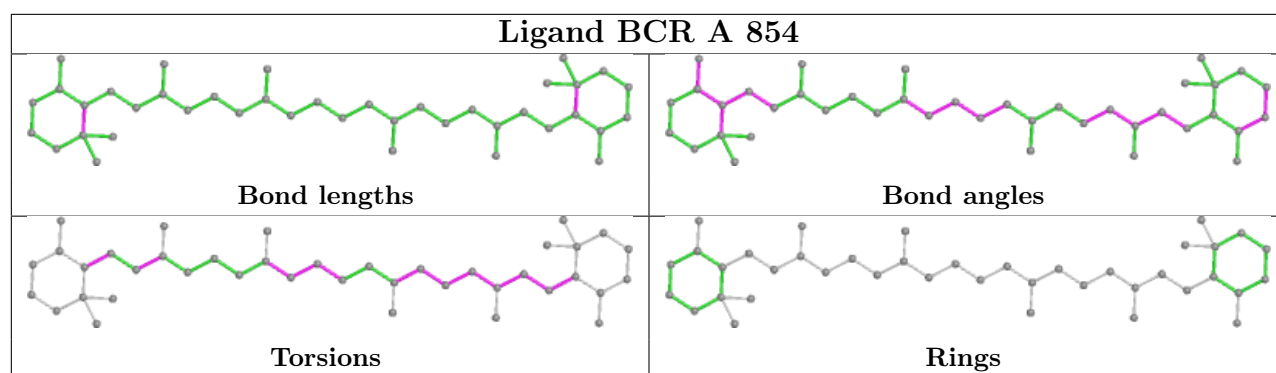
Rings

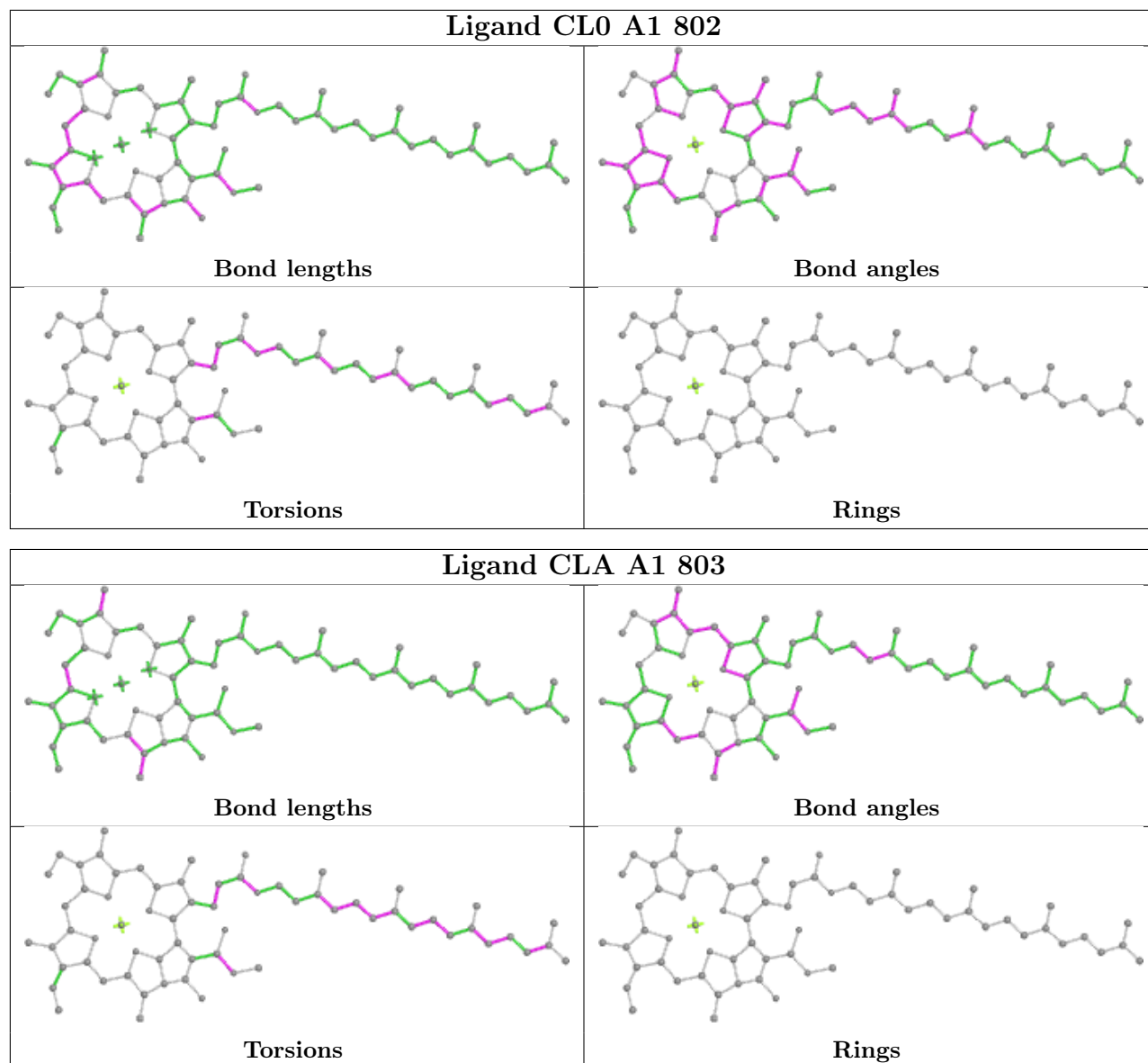


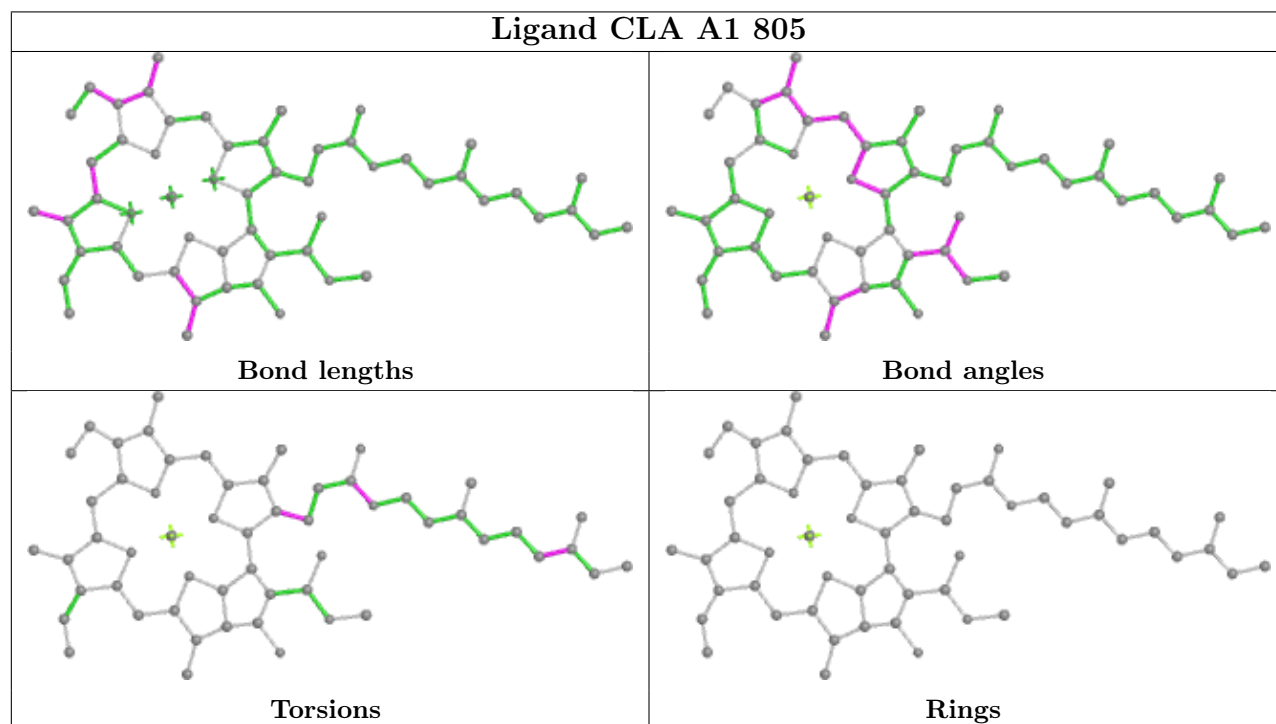
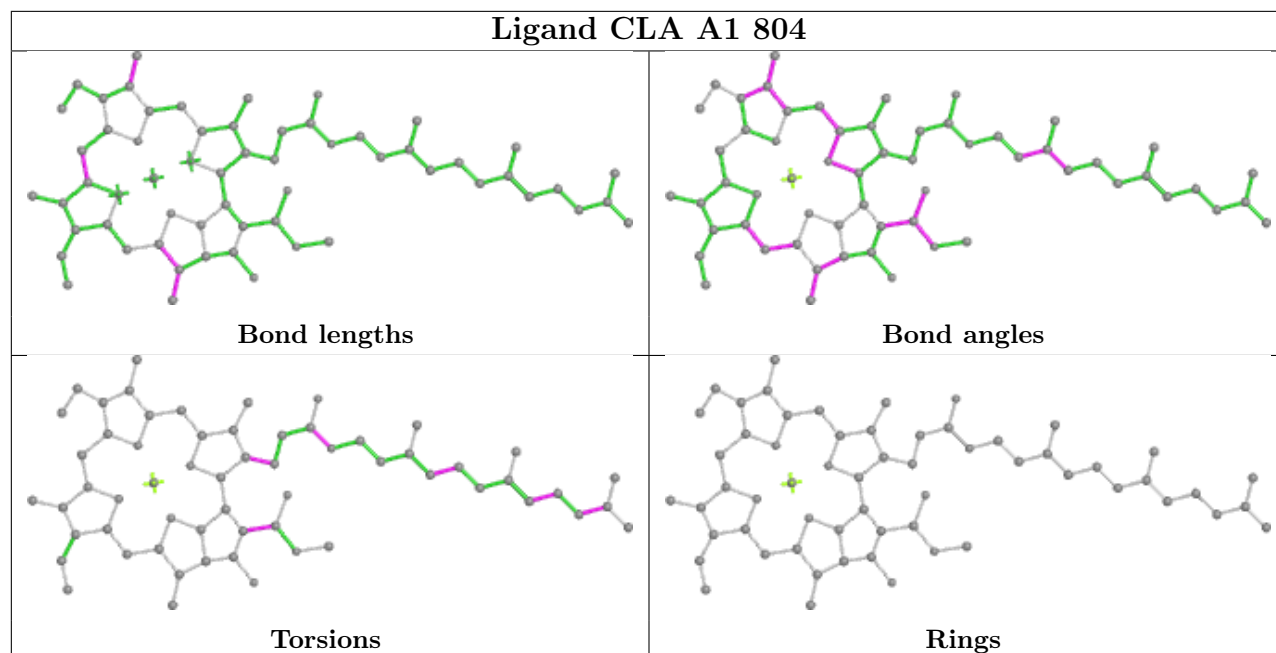


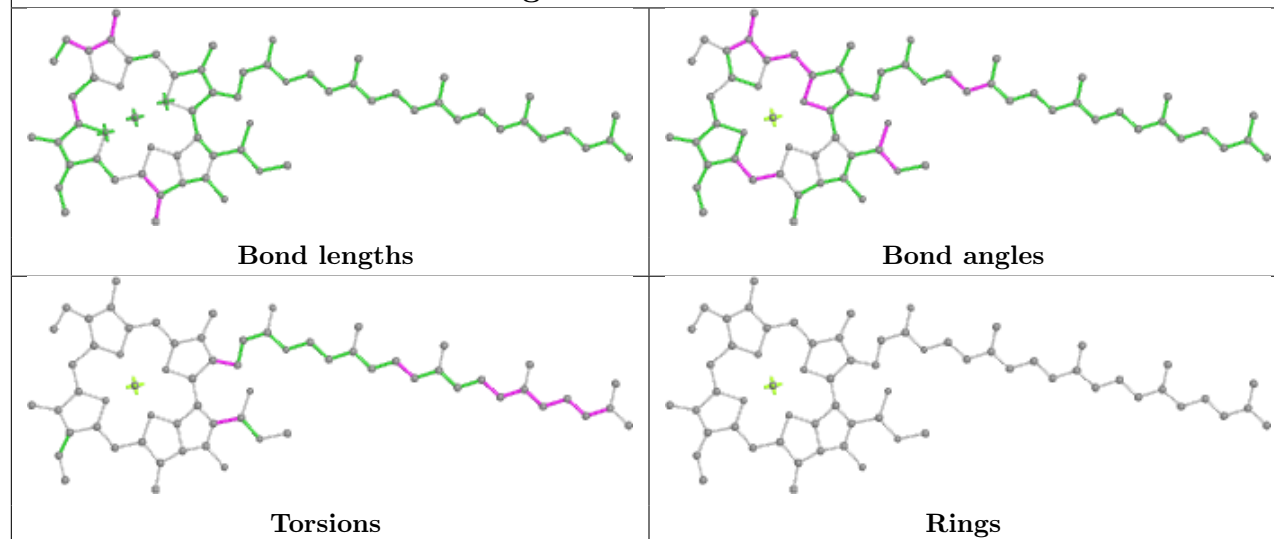
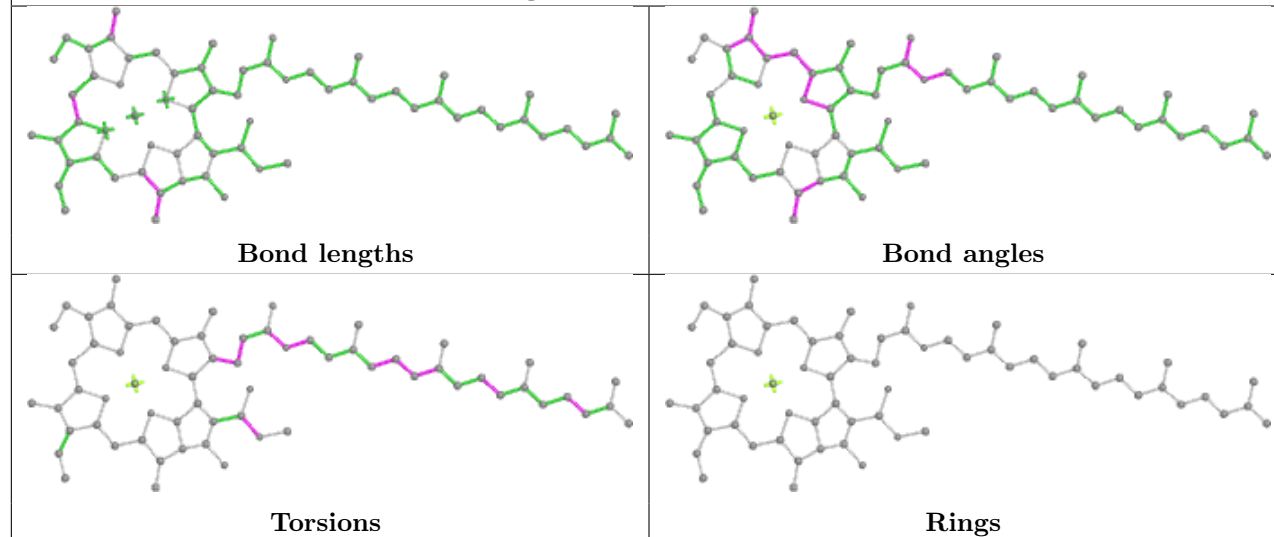




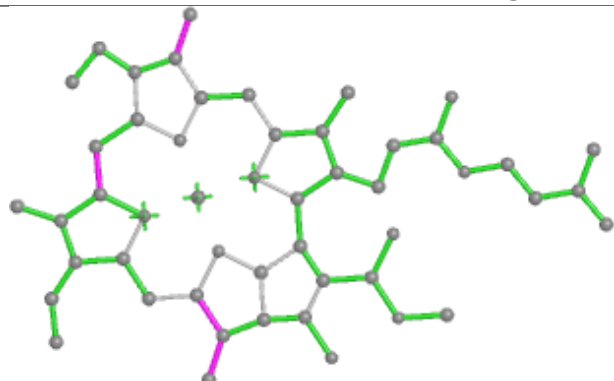




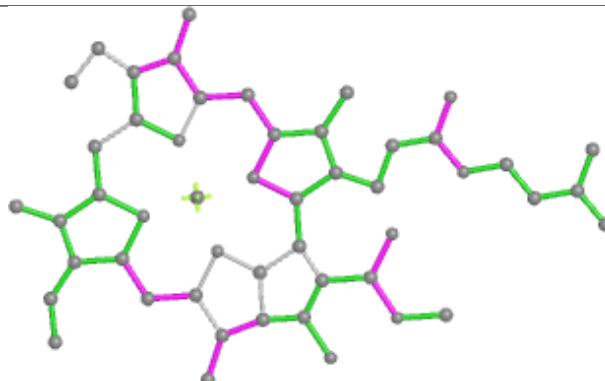


Ligand CLA A1 806**Ligand CLA A1 807**

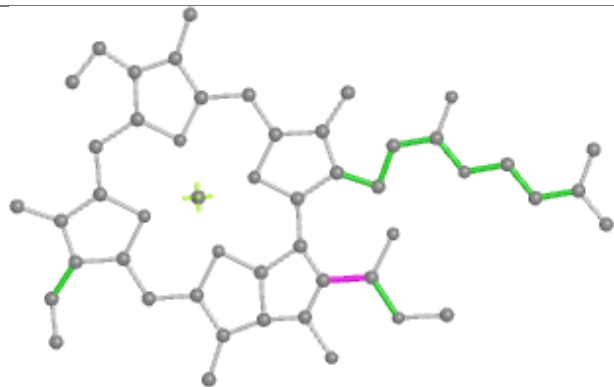
Ligand CLA A1 808



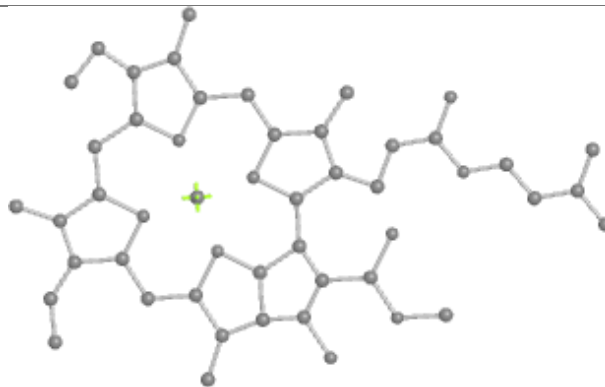
Bond lengths



Bond angles

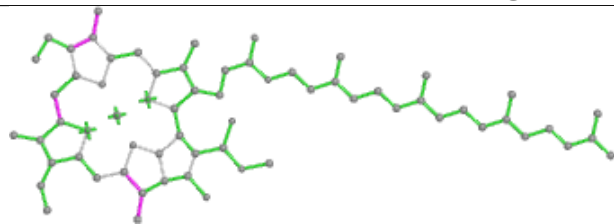


Torsions

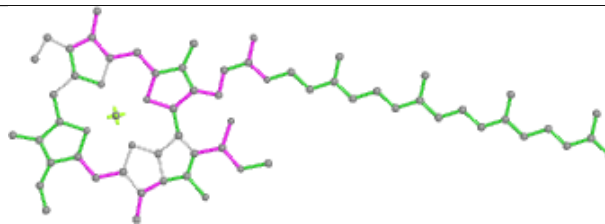


Rings

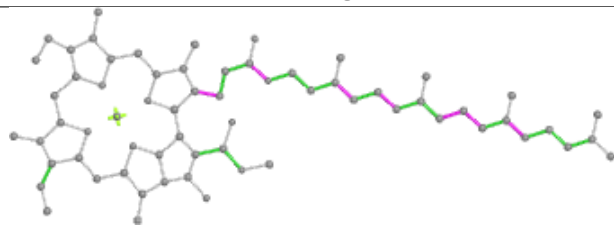
Ligand CLA A1 809



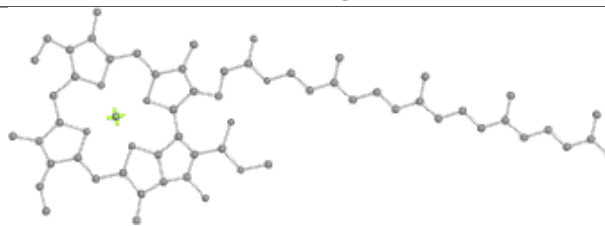
Bond lengths



Bond angles

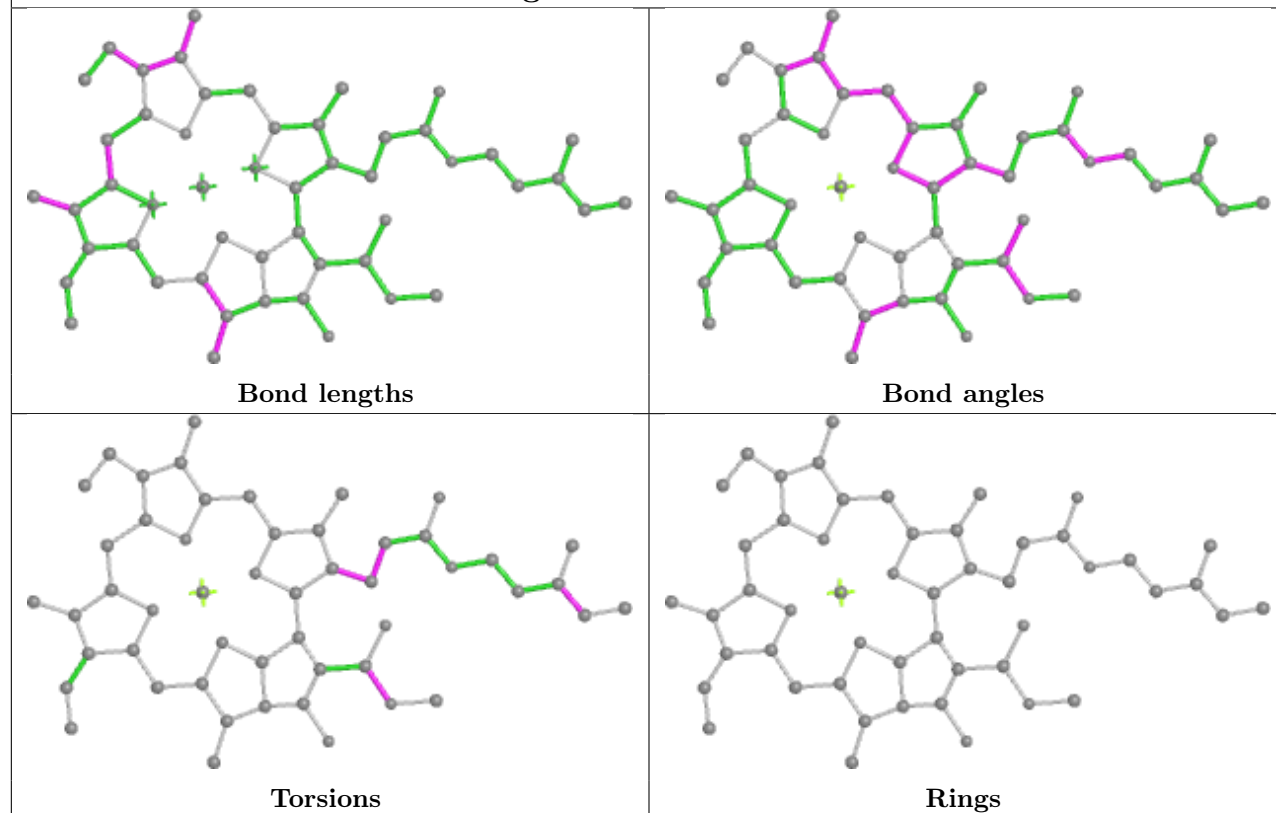


Torsions

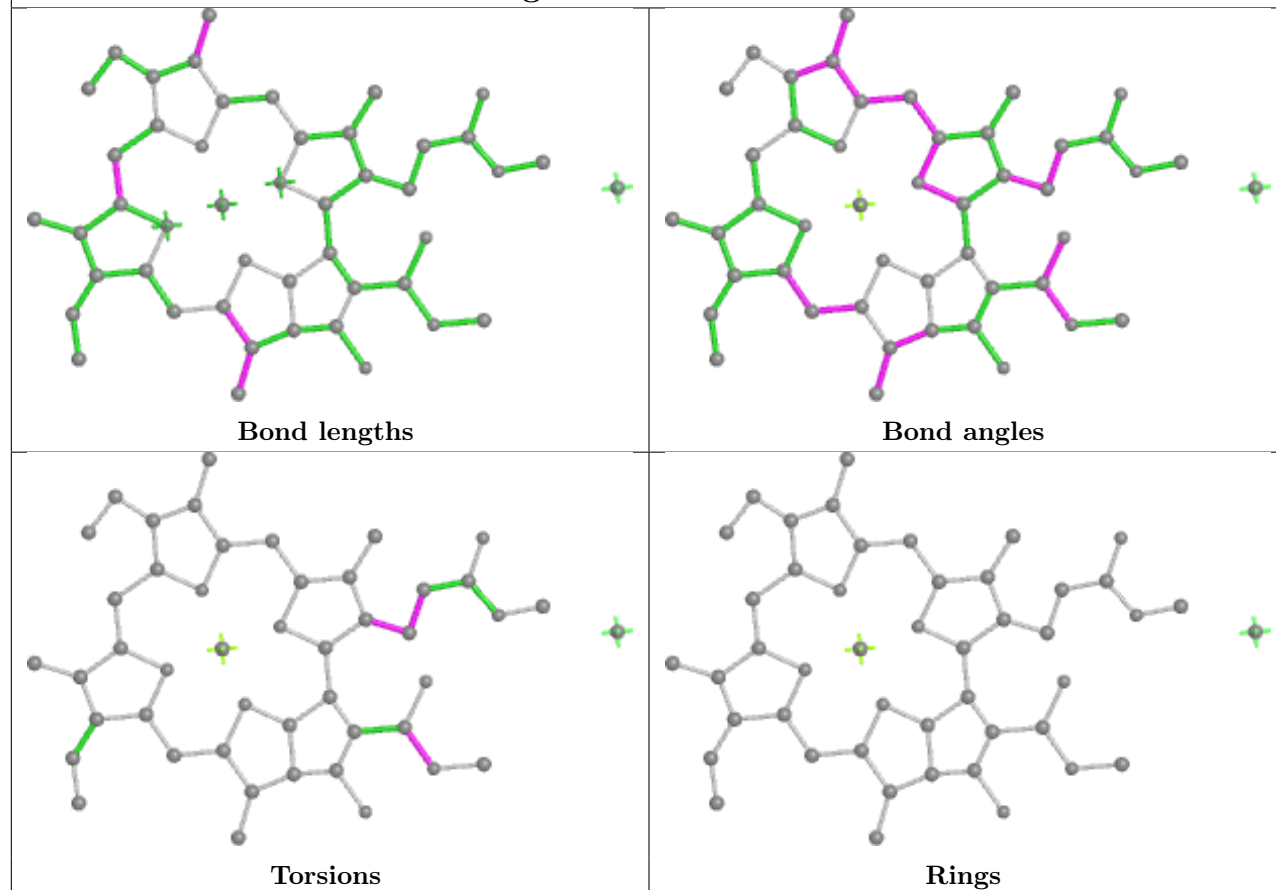


Rings

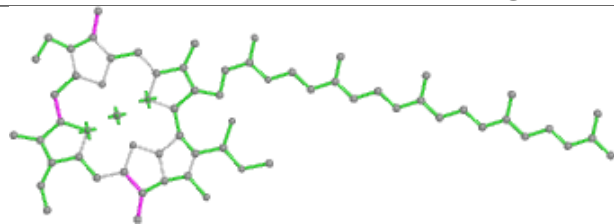
Ligand CLA A1 810



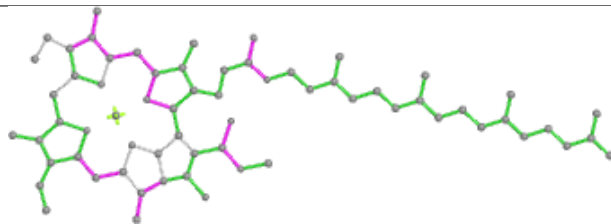
Ligand CLA A1 811



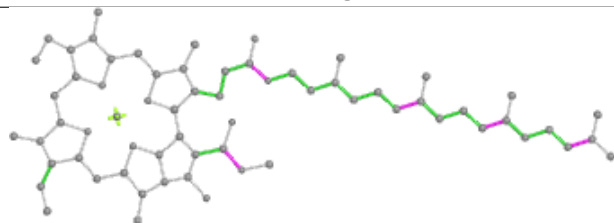
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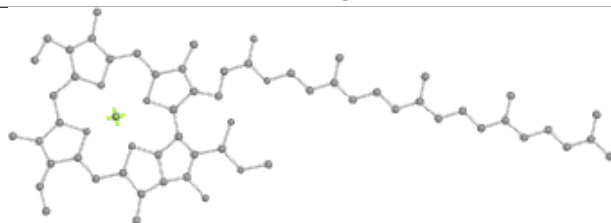
Bond lengths



Bond angles

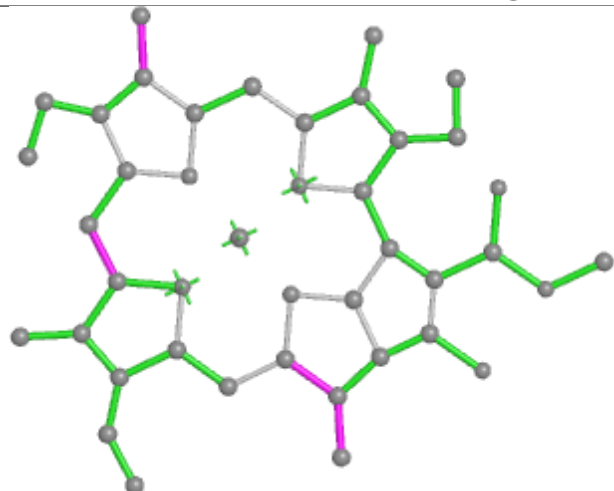


Torsions

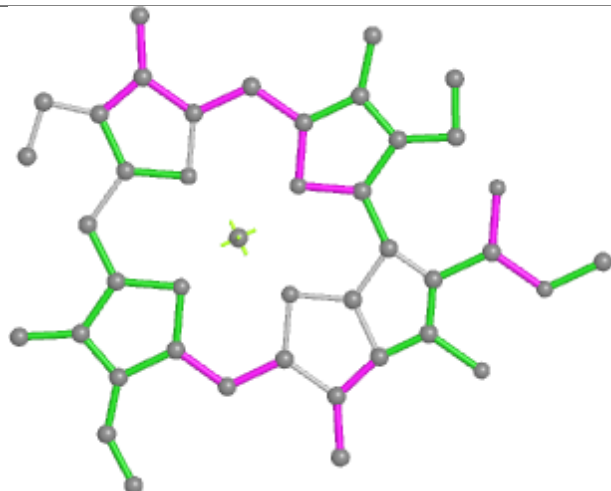


Rings

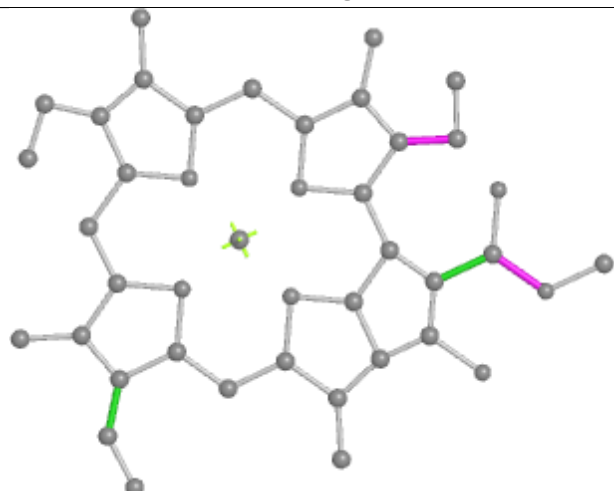
Ligand CLA A1 813



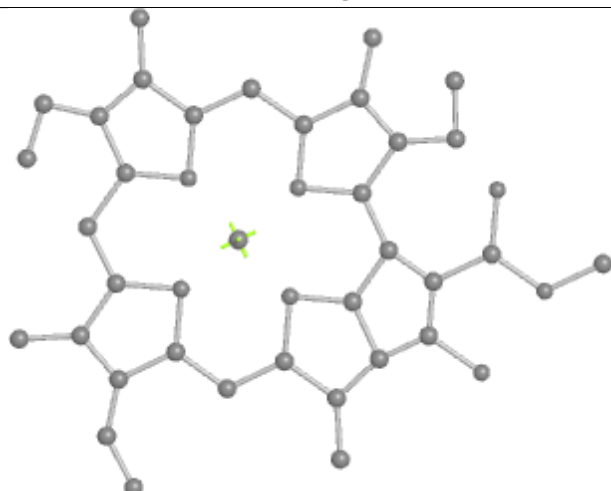
Bond lengths



Bond angles

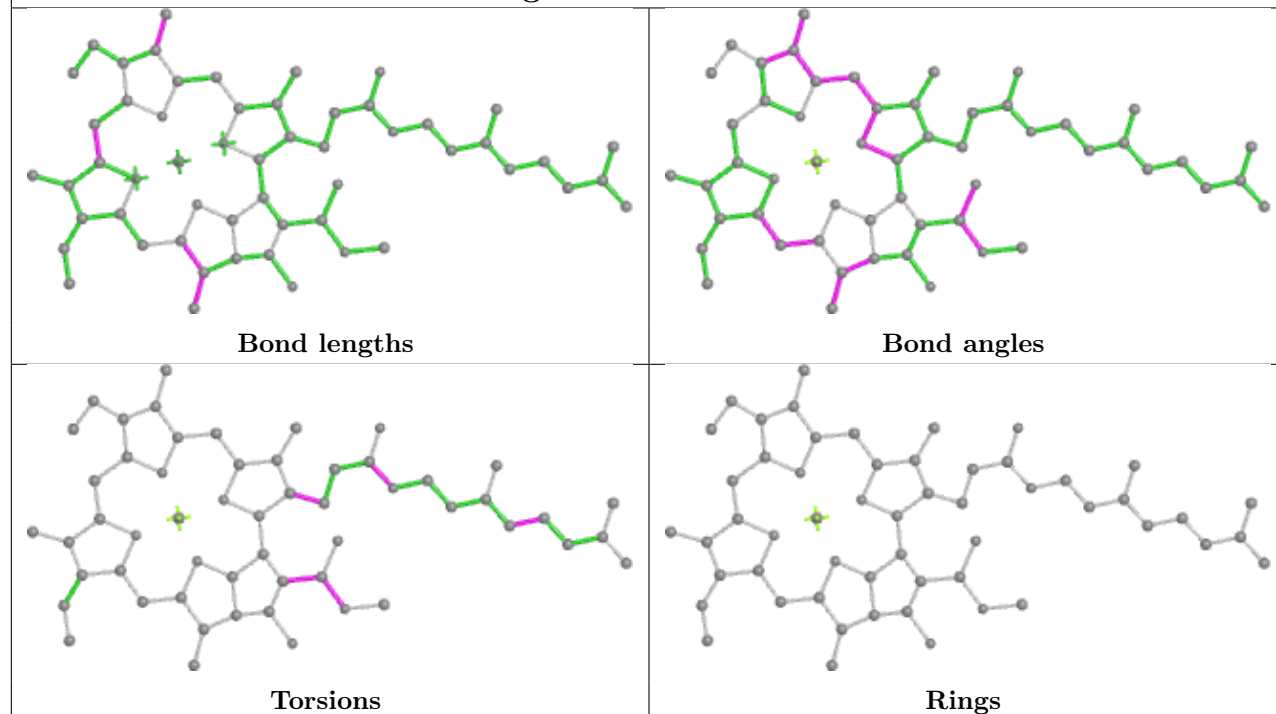


Torsions

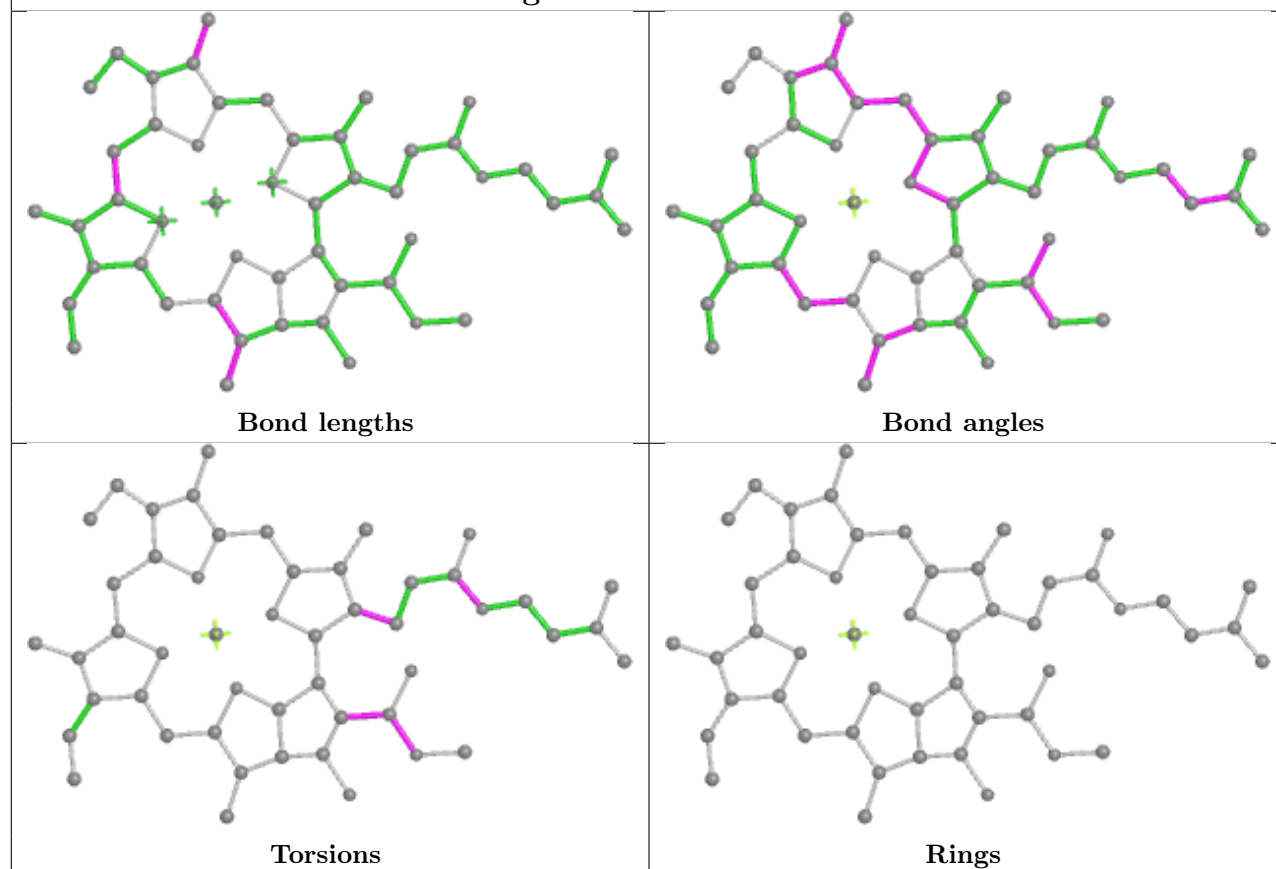


Rings

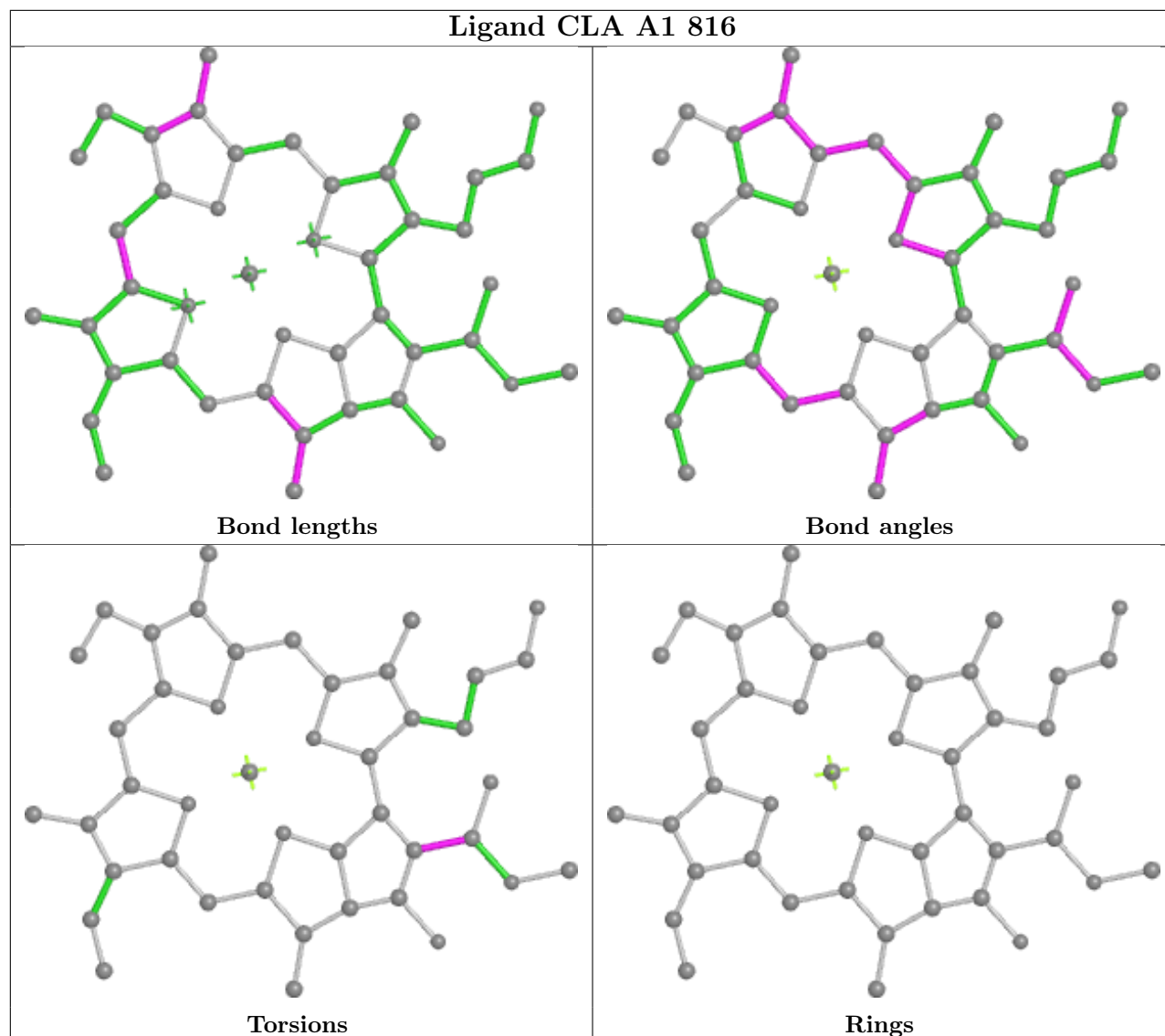
Ligand CLA A1 814



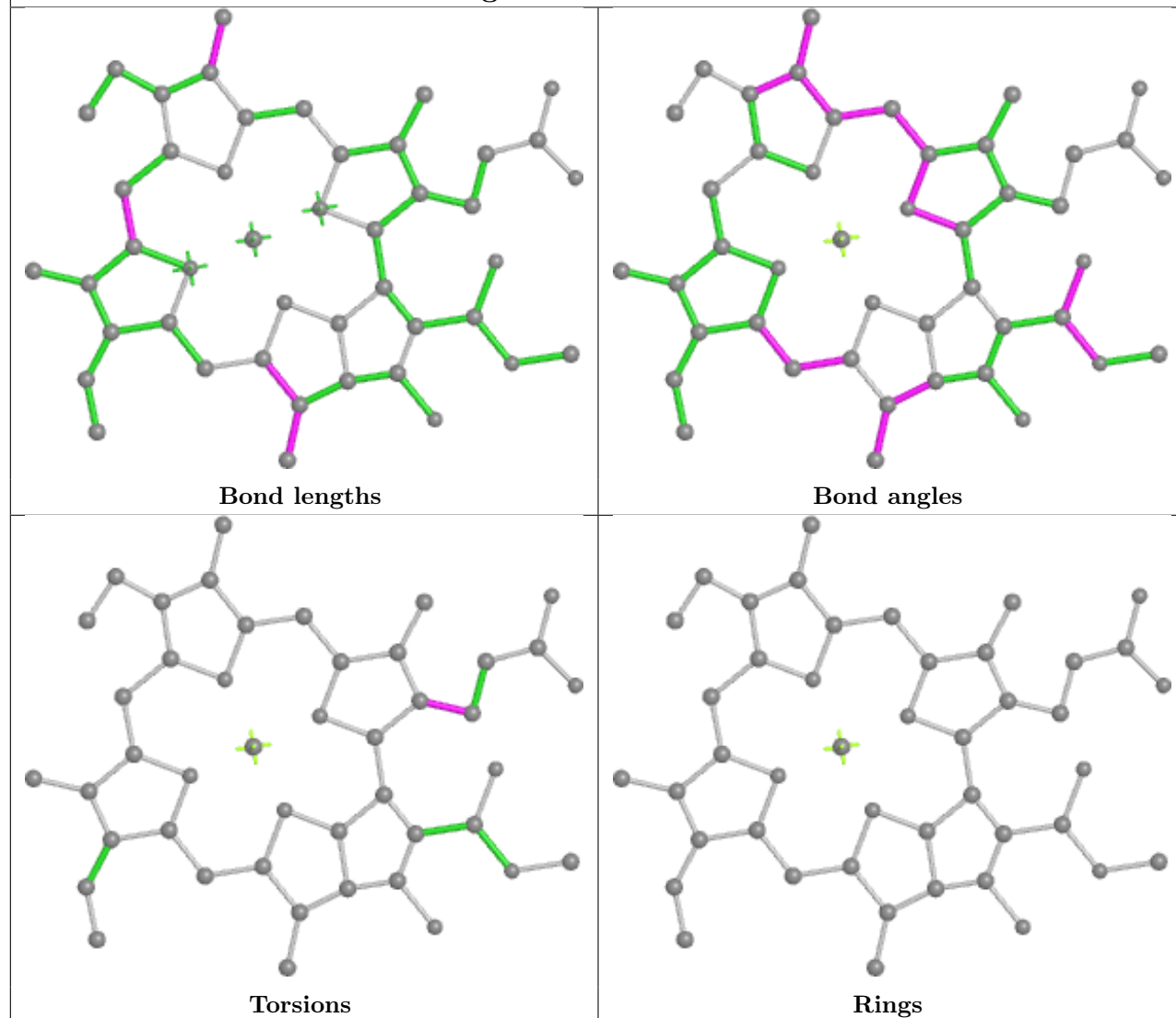
Ligand CLA A1 815



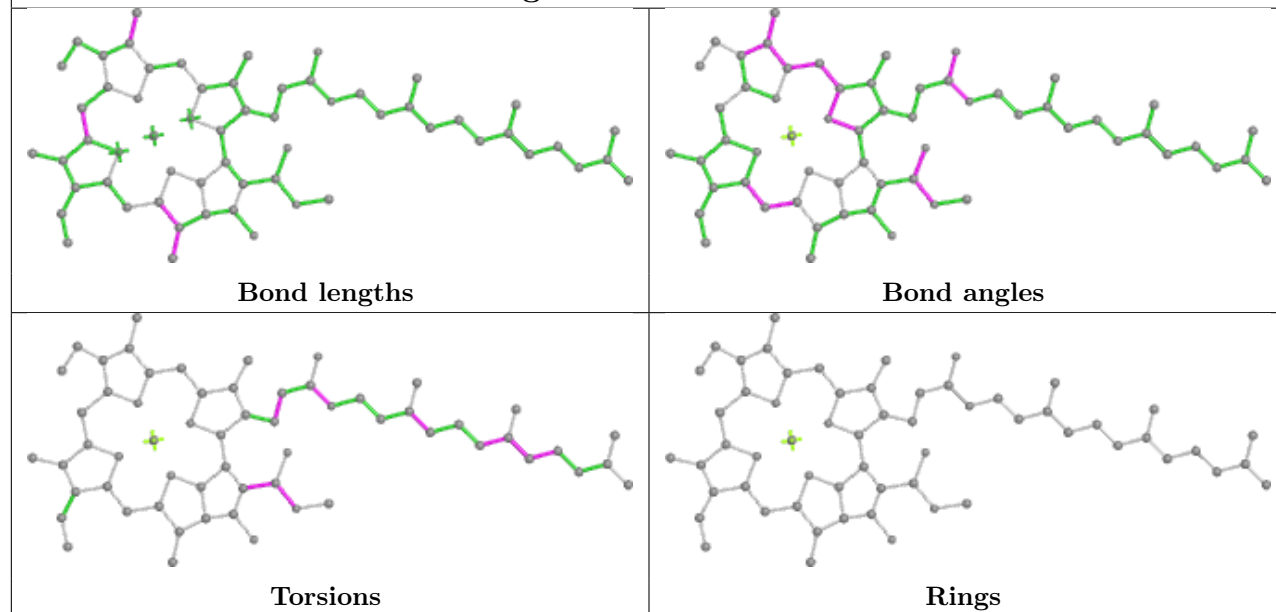
Ligand CLA A1 816

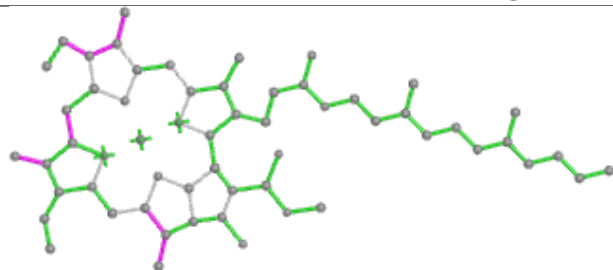
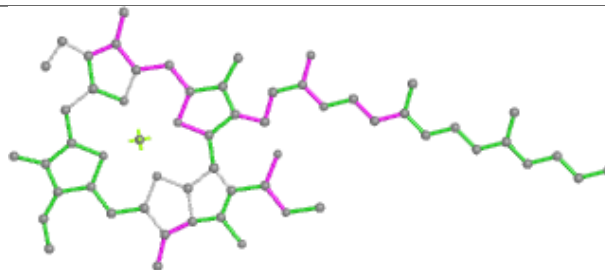
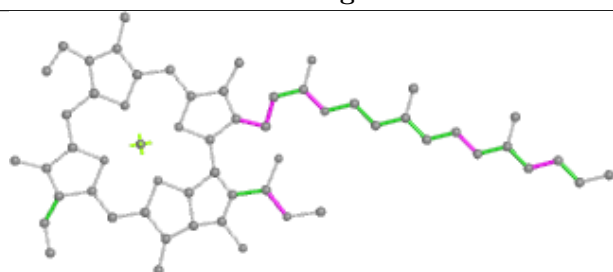
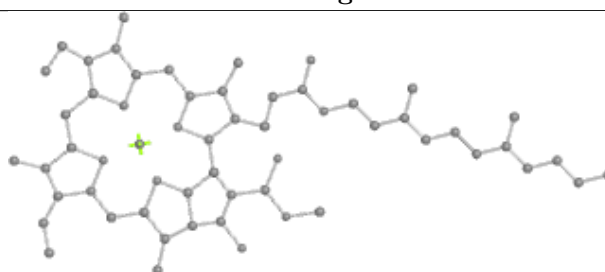
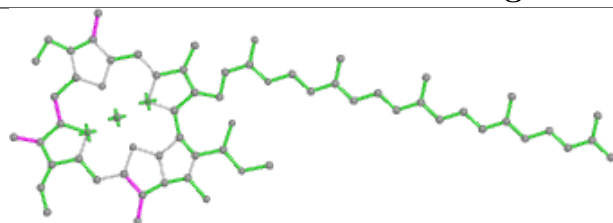
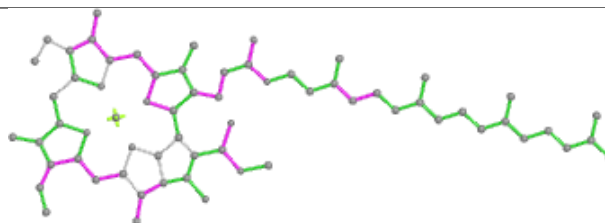
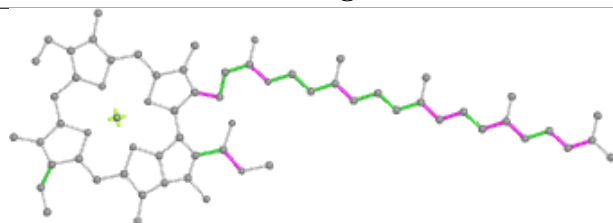
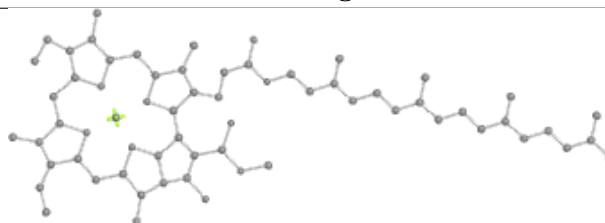


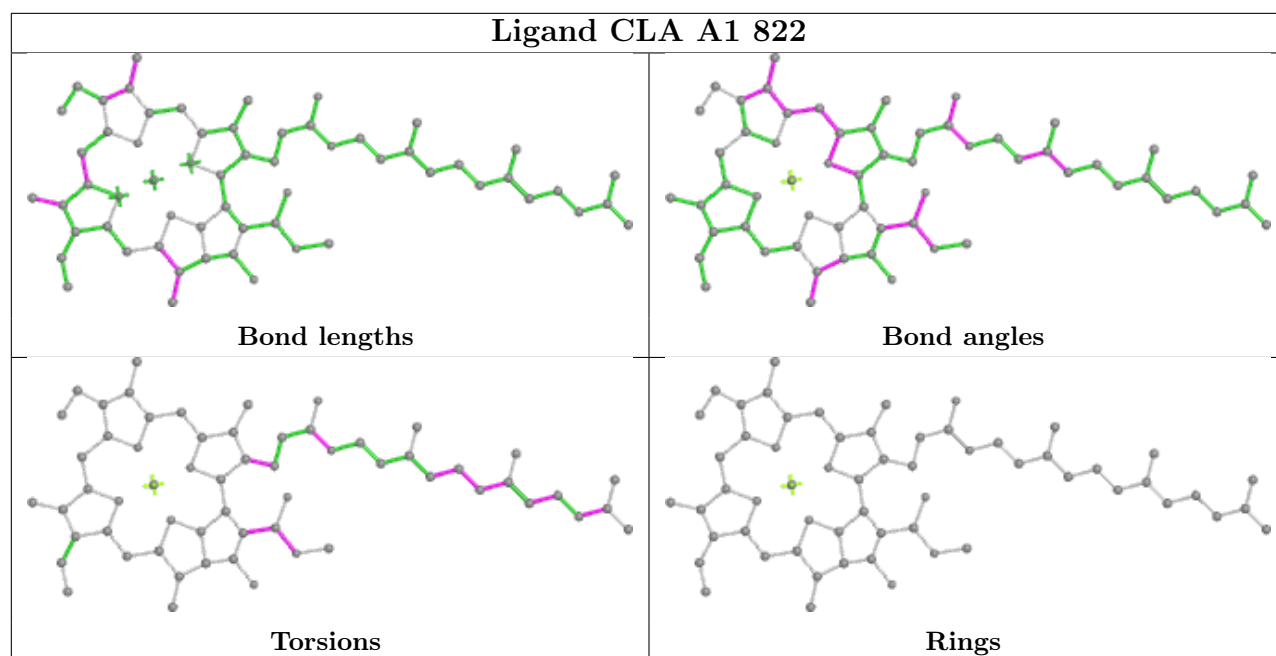
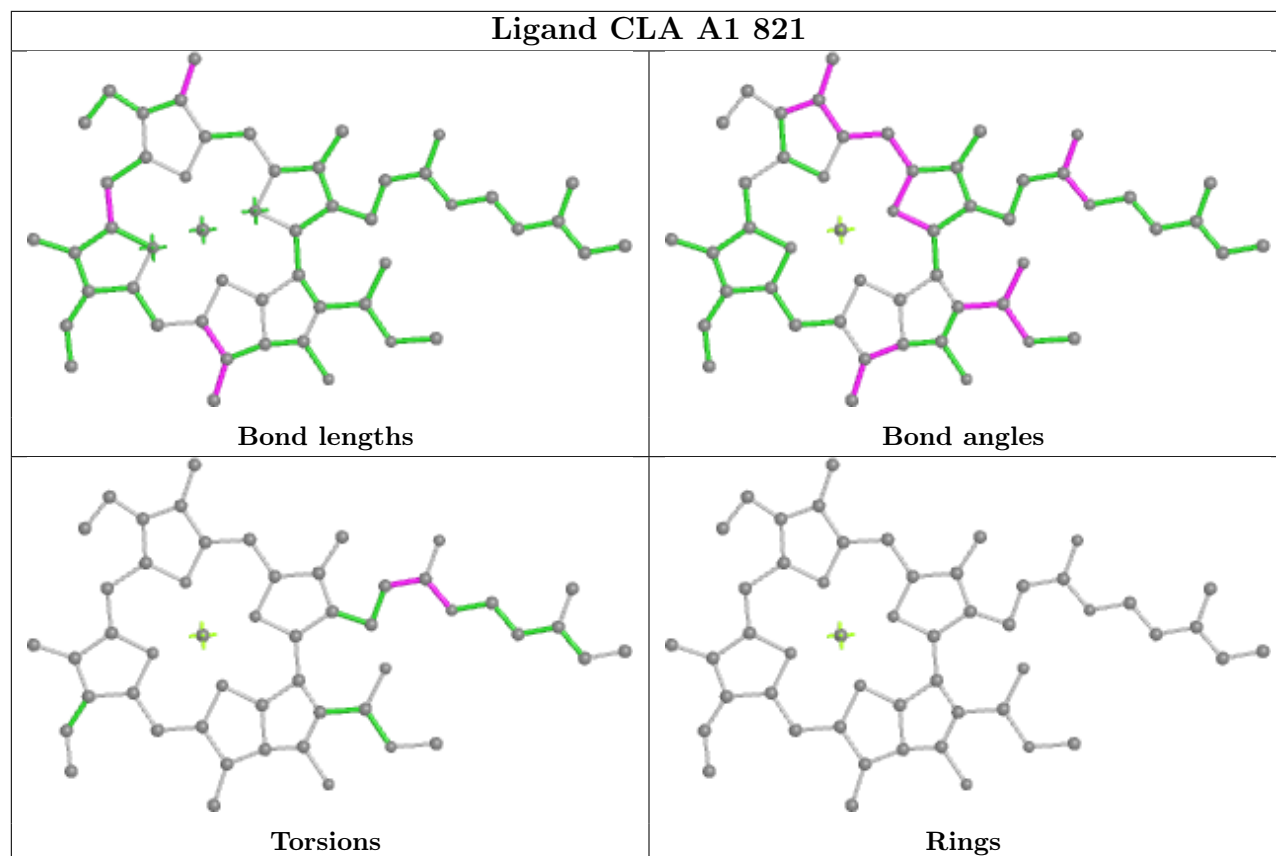
Ligand CLA A1 817



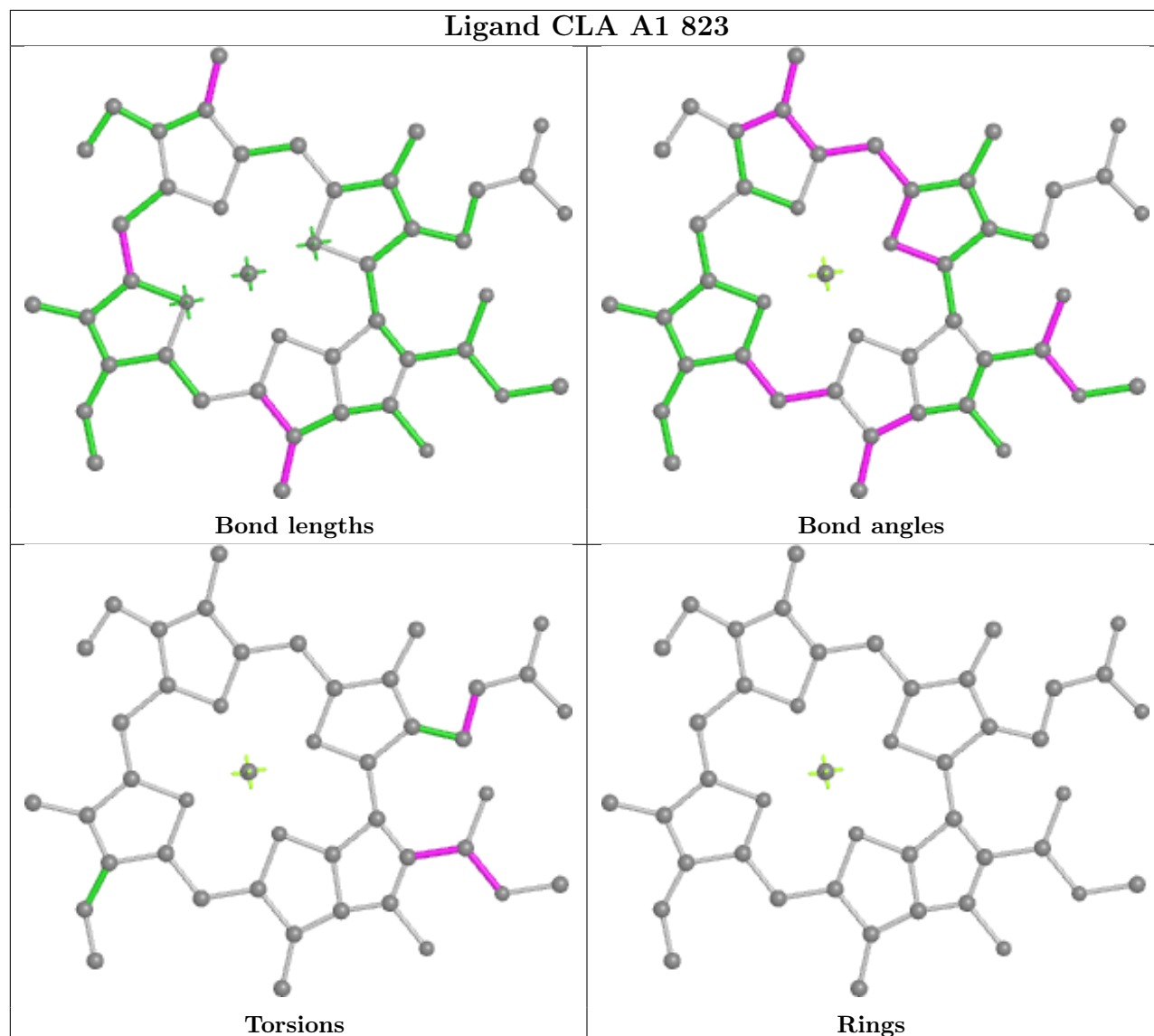
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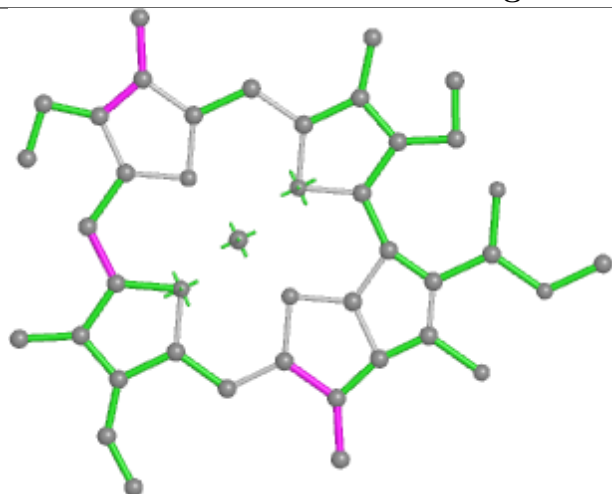
Ligand CLA A1 819**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A1 820****Bond lengths****Bond angles****Torsions****Rings**



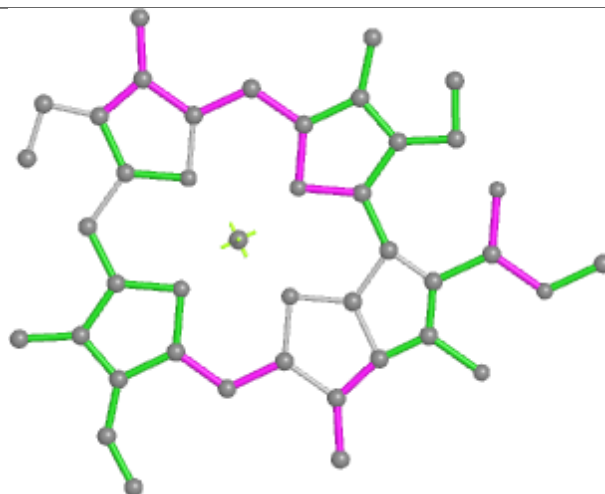
Ligand CLA A1 823



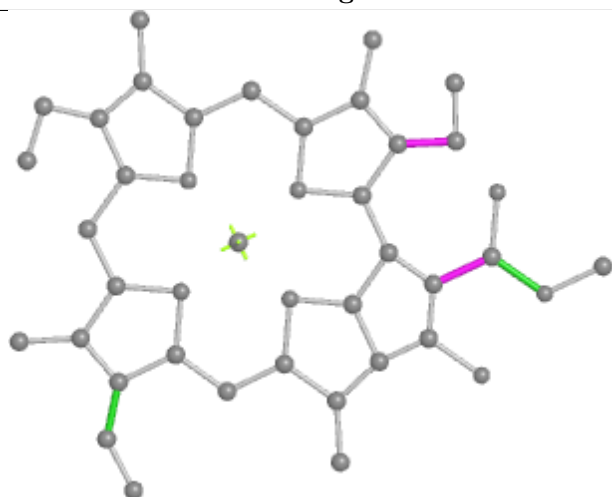
Ligand CLA A1 824



Bond lengths



Bond angles

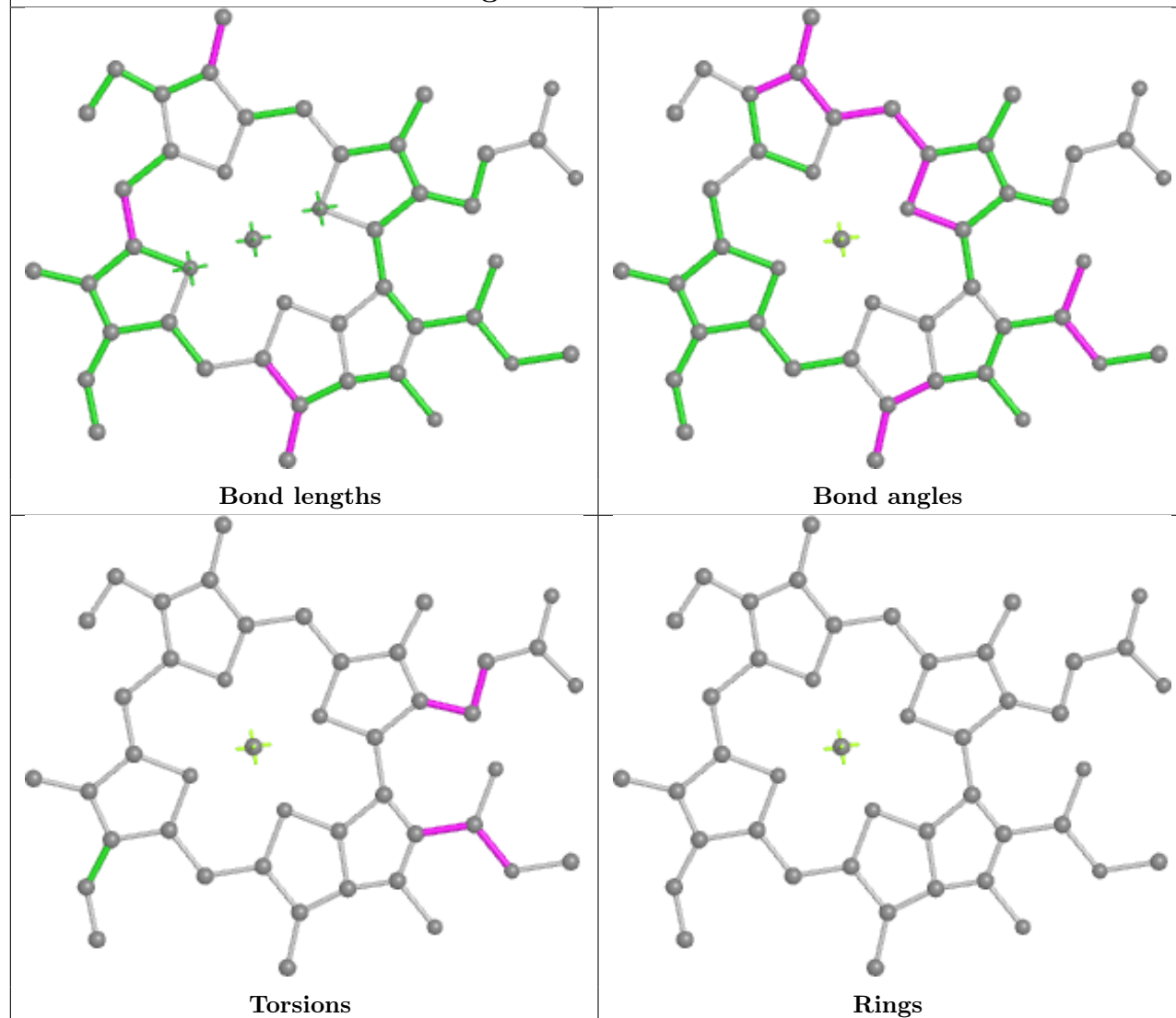


Torsions

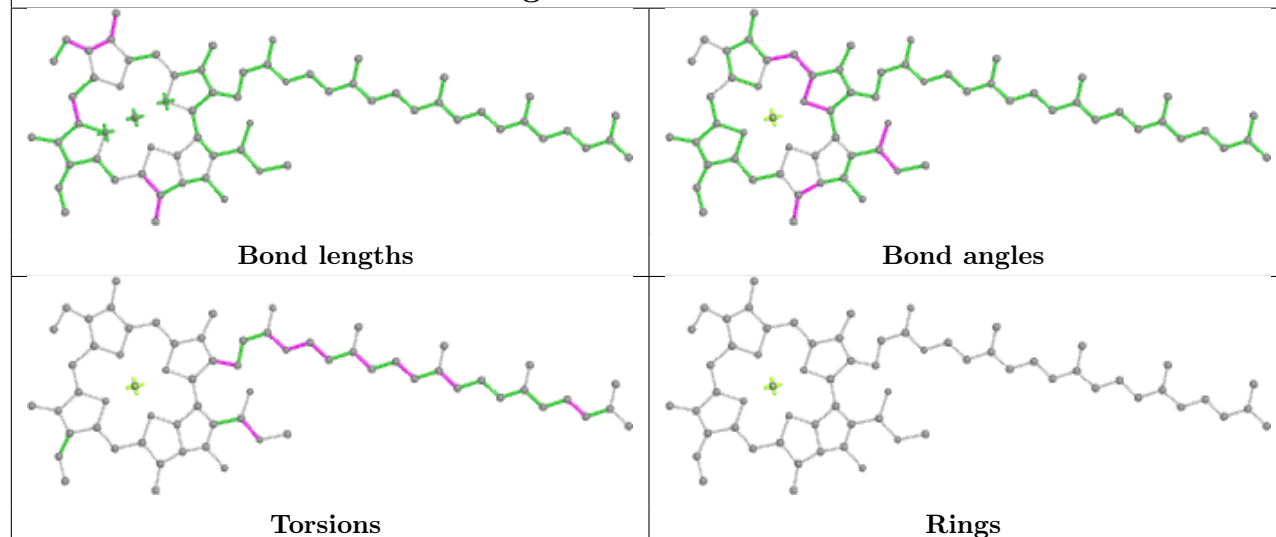


Rings

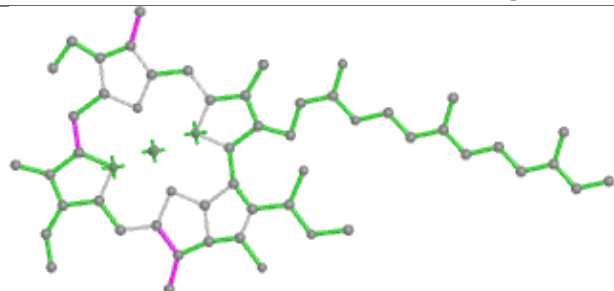
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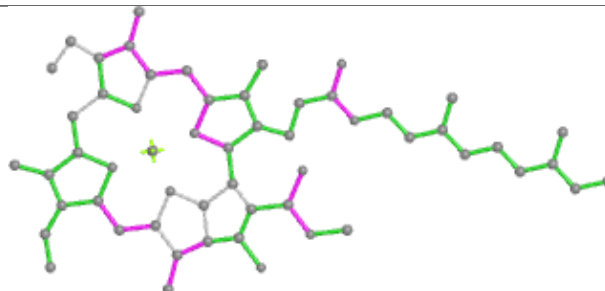
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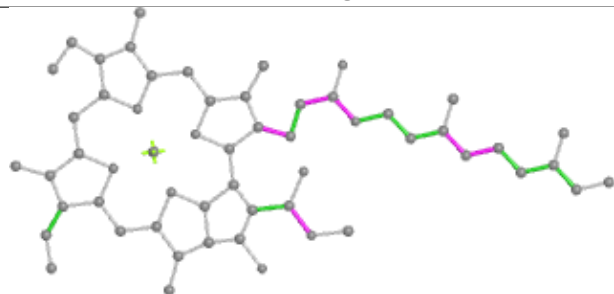
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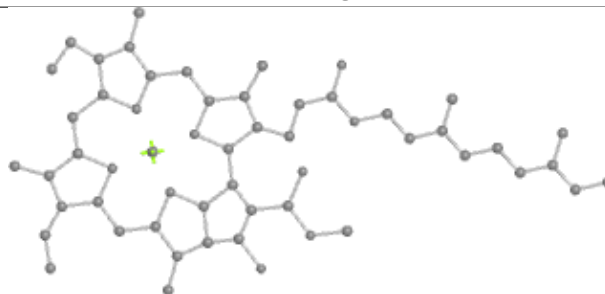
Bond lengths



Bond angles

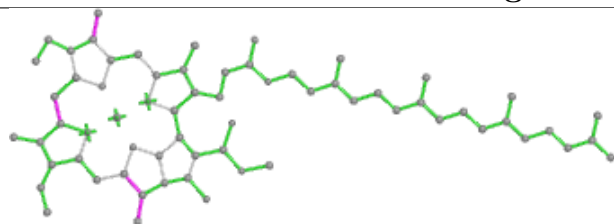


Torsions

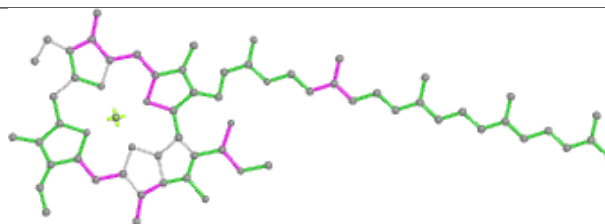


Rings

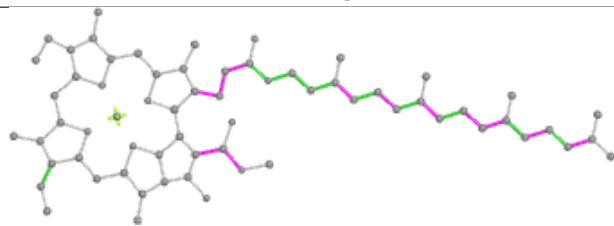
Ligand CLA A1 828



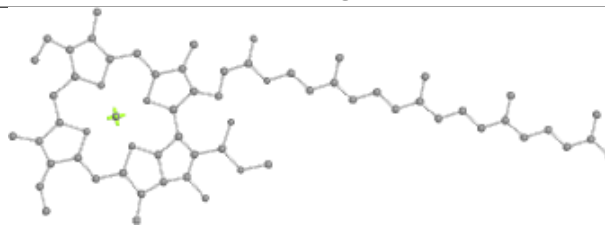
Bond lengths



Bond angles

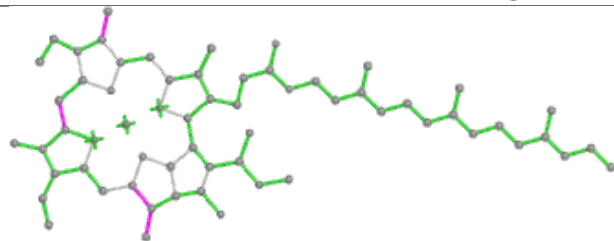


Torsions

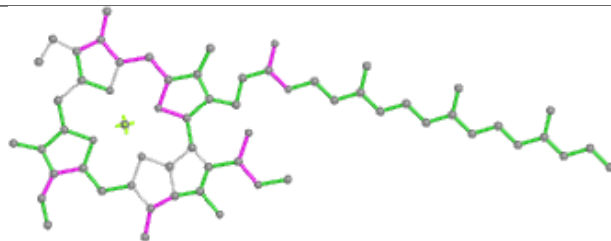


Rings

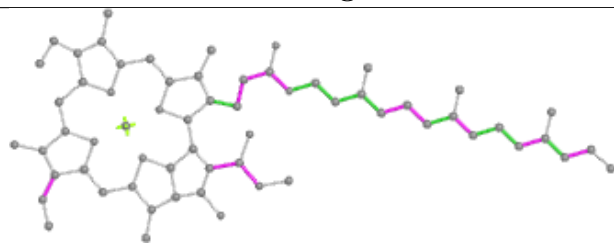
Ligand CLA A1 829



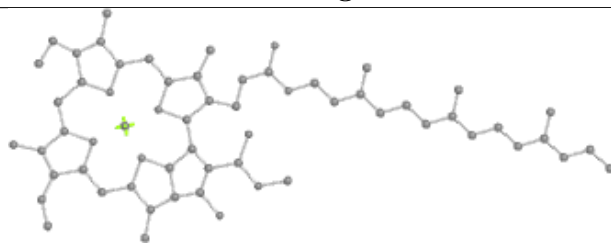
Bond lengths



Bond angles

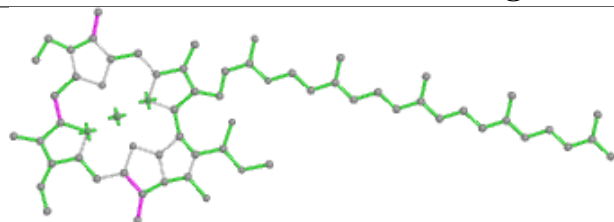


Torsions

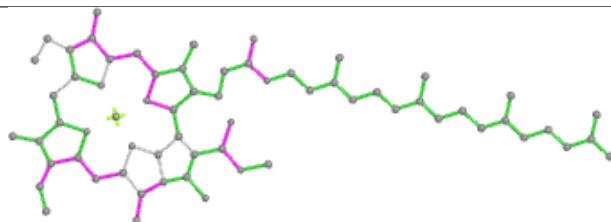


Rings

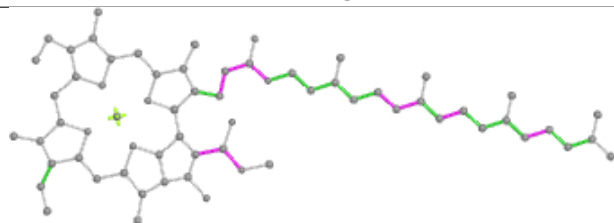
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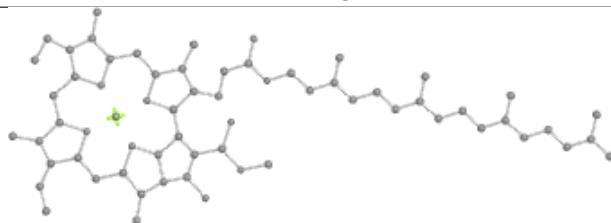
Bond lengths



Bond angles

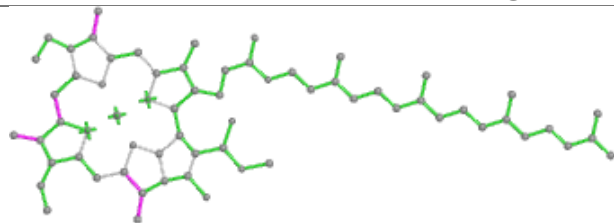


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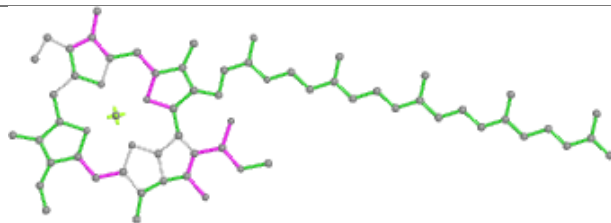


Rings

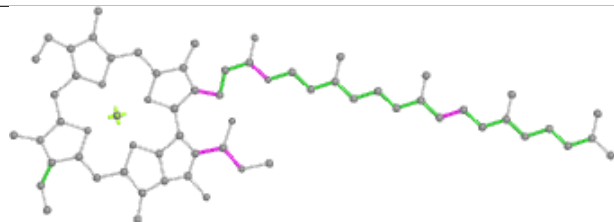
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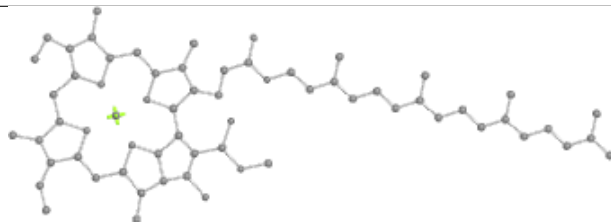
Bond lengths



Bond angles

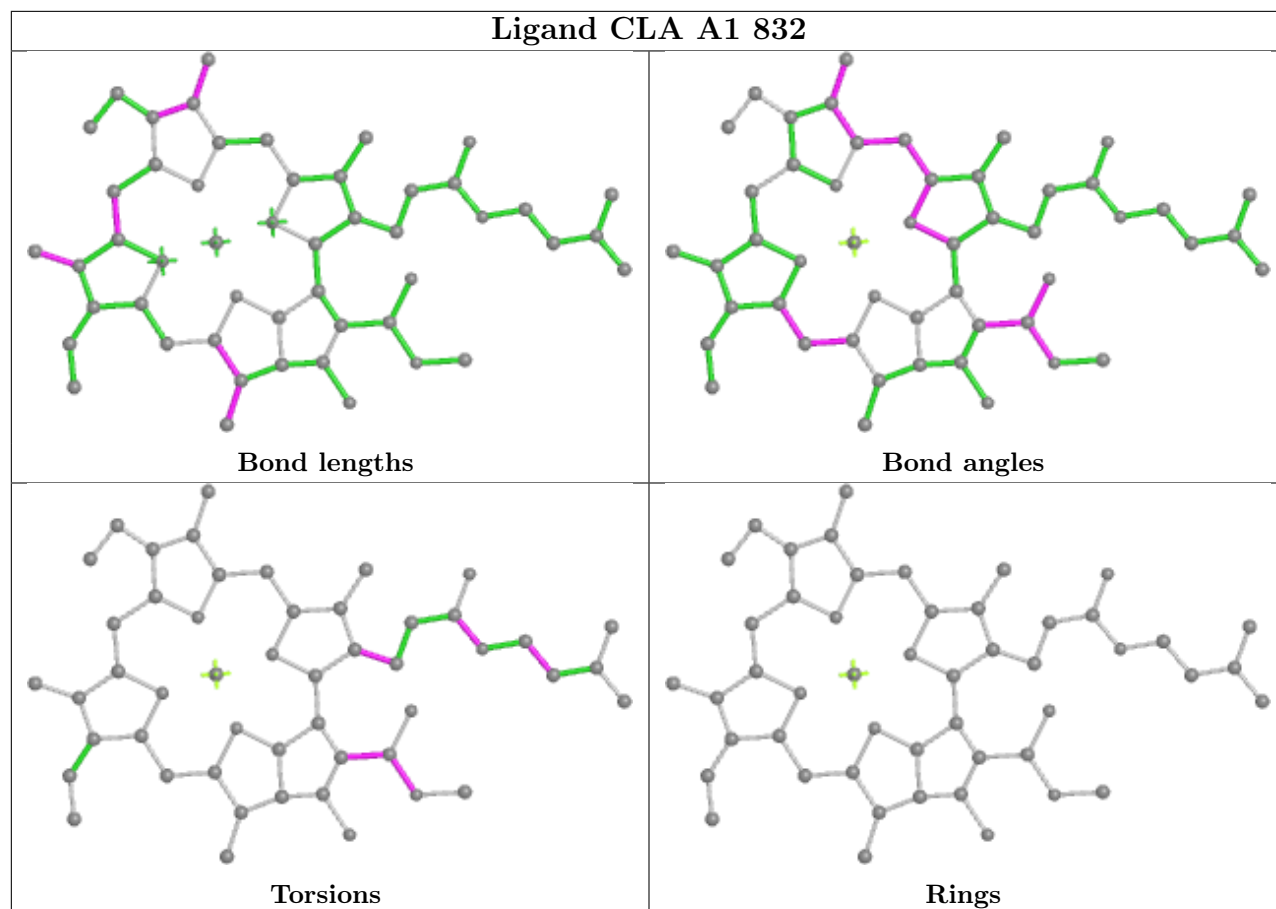


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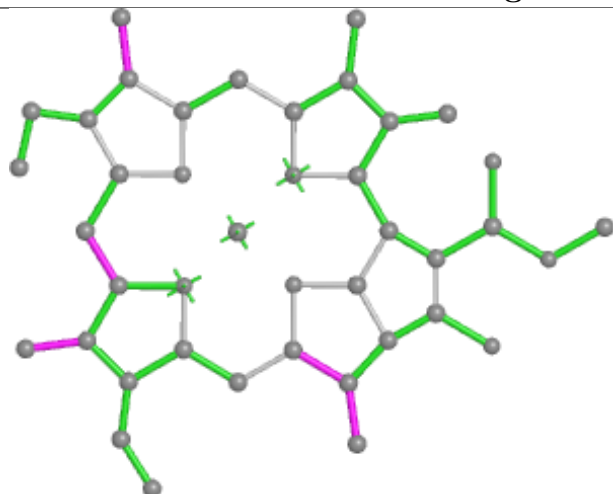


Rings

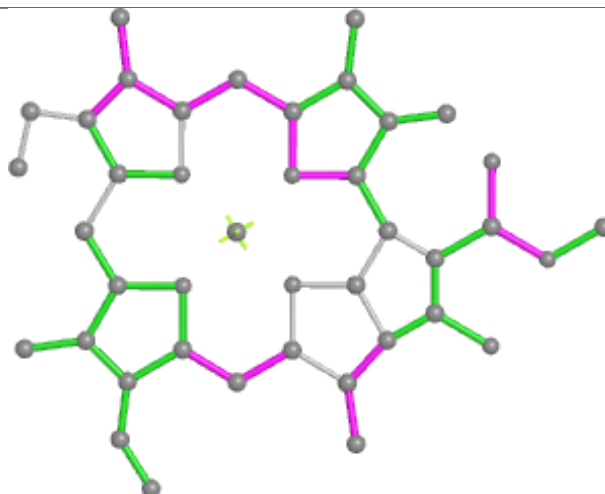
Ligand CLA A1 832



Ligand CLA A1 833



Bond lengths



Bond angles

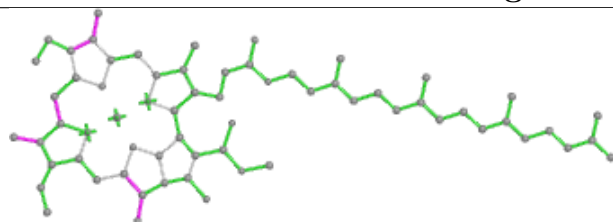


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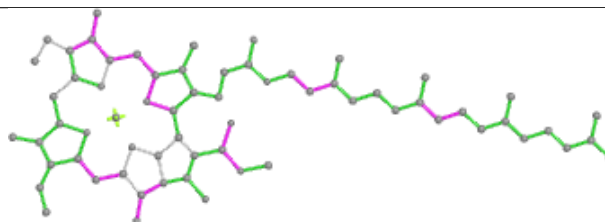


Rings

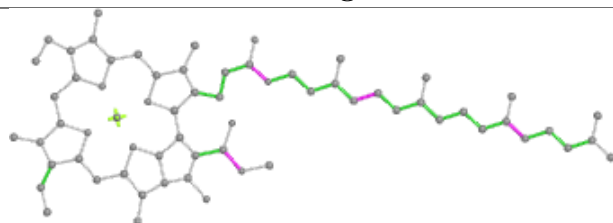
Ligand CLA A1 834



Bond lengths



Bond angles

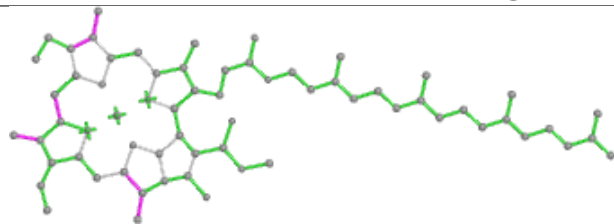


Torsions

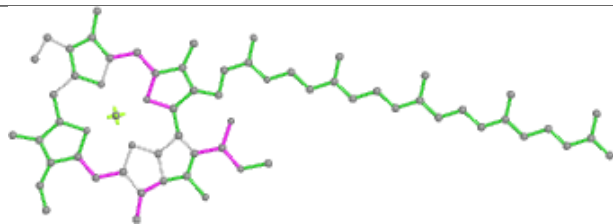


Rings

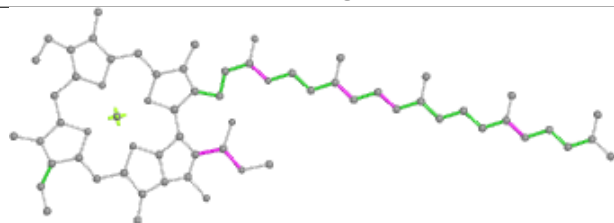
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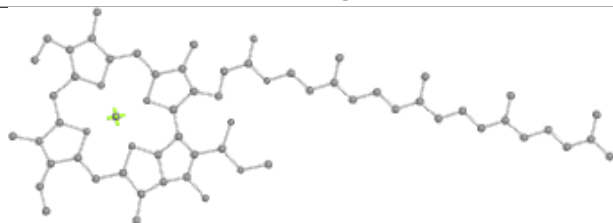
Bond lengths



Bond angles

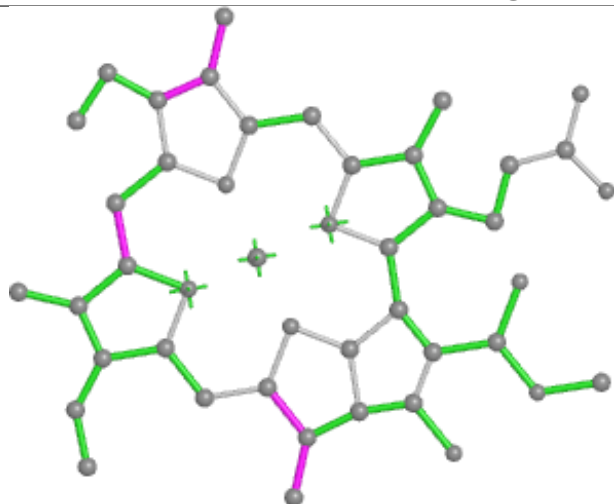


Torsions

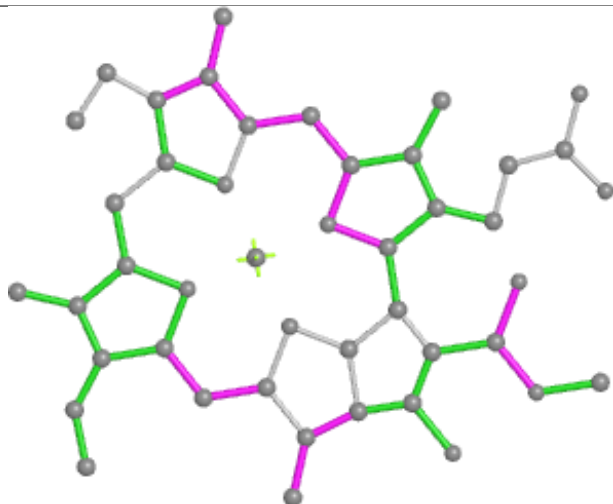


Rings

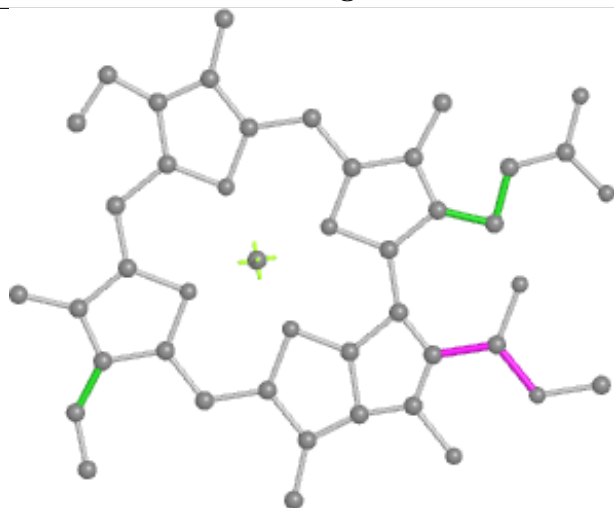
Ligand CLA A1 836



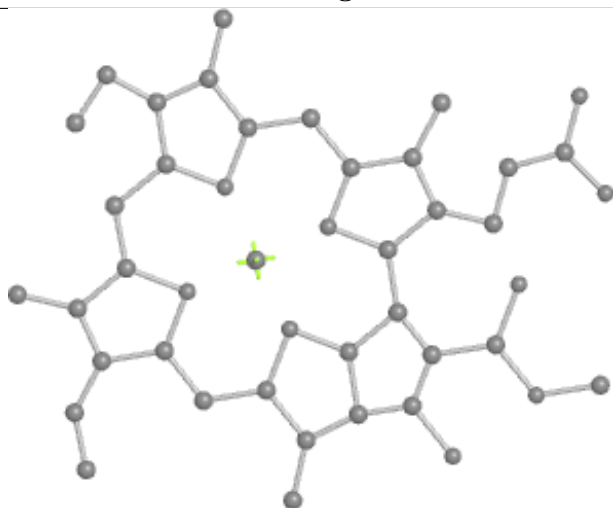
Bond lengths



Bond angles

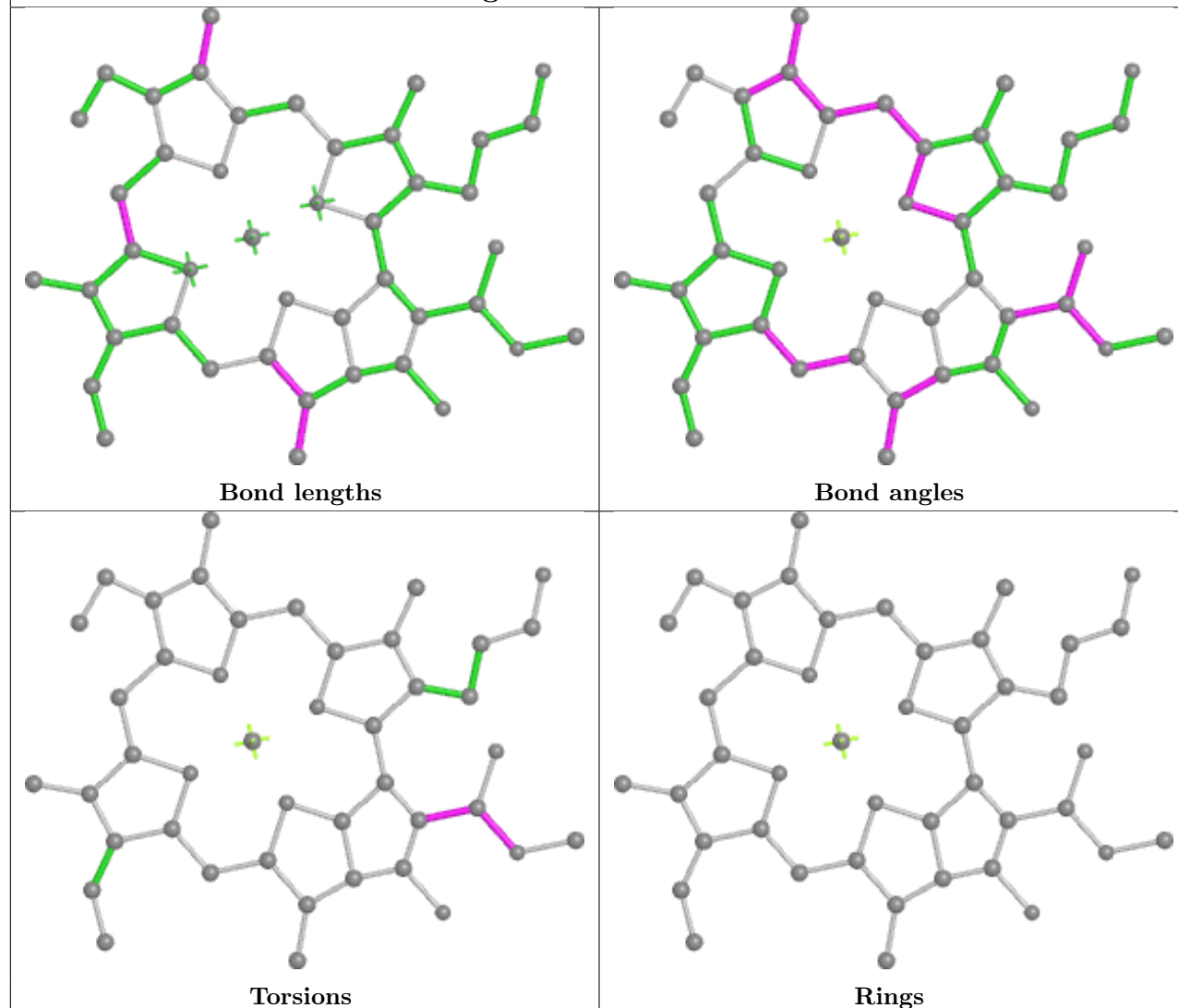


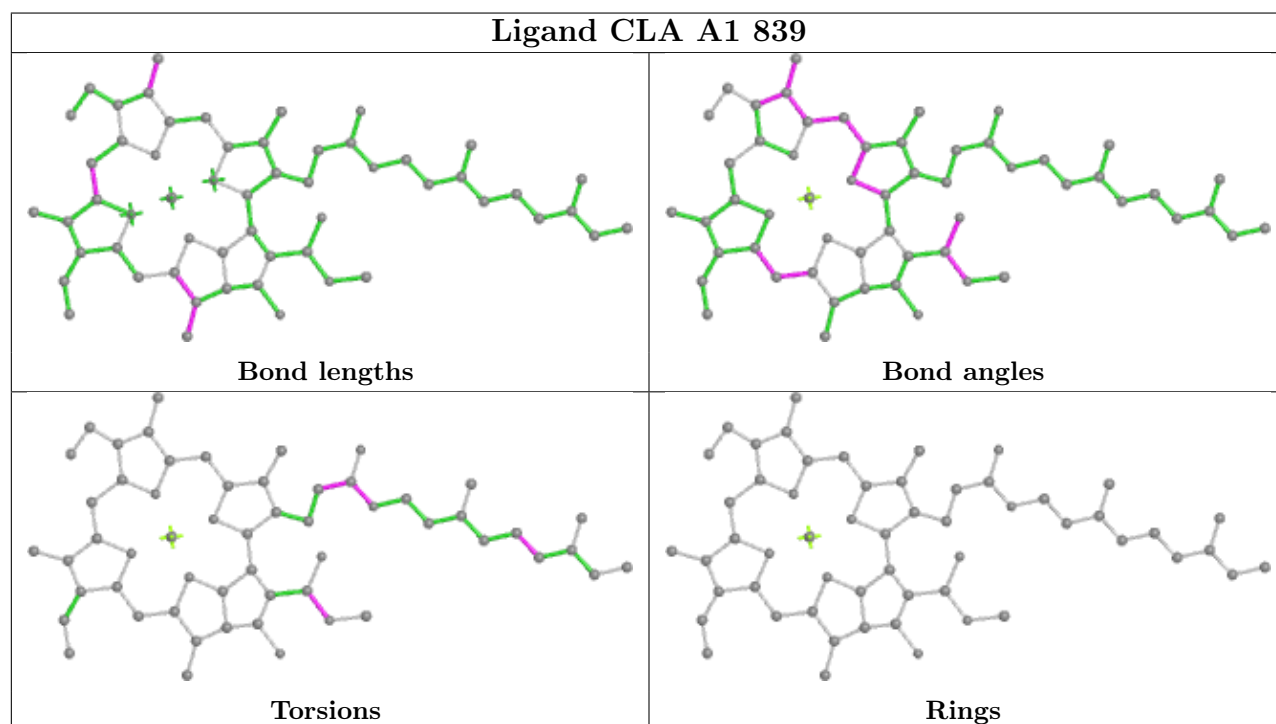
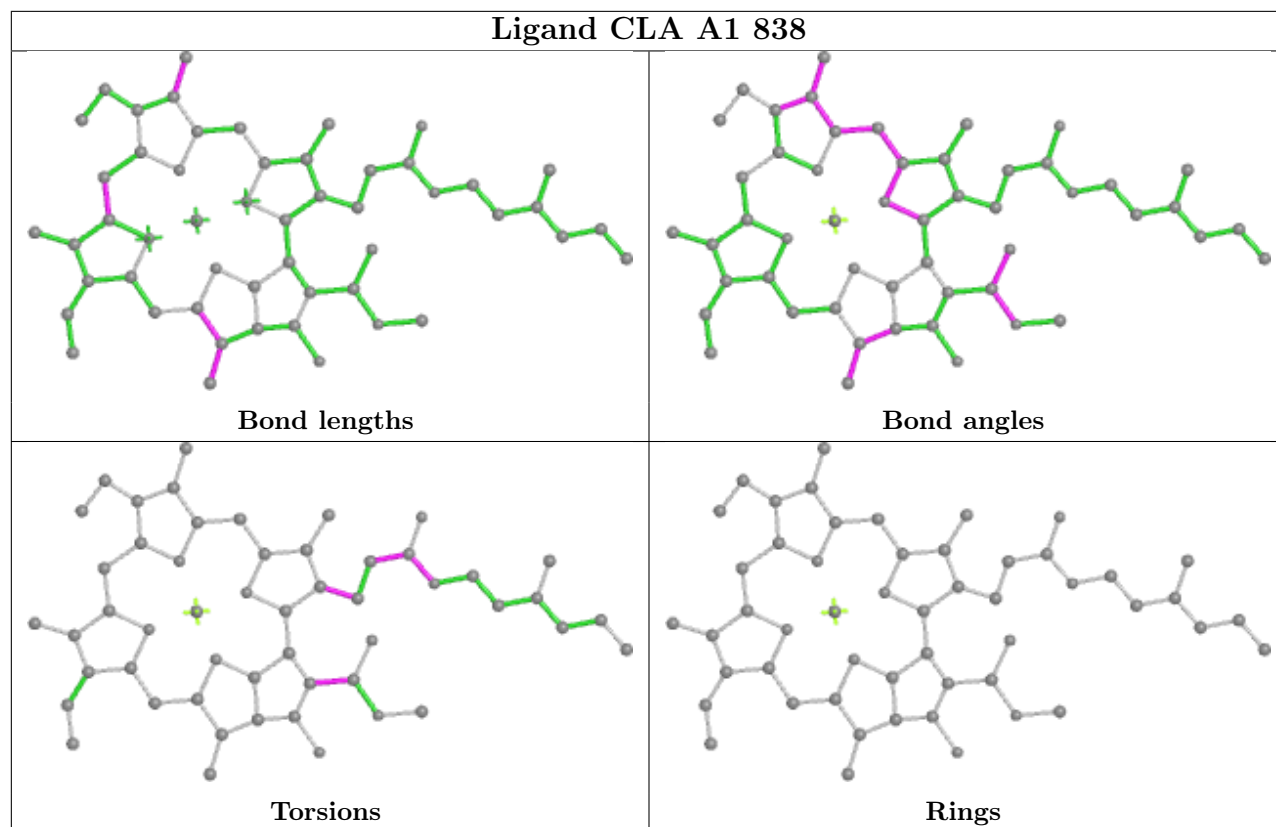
Torsions



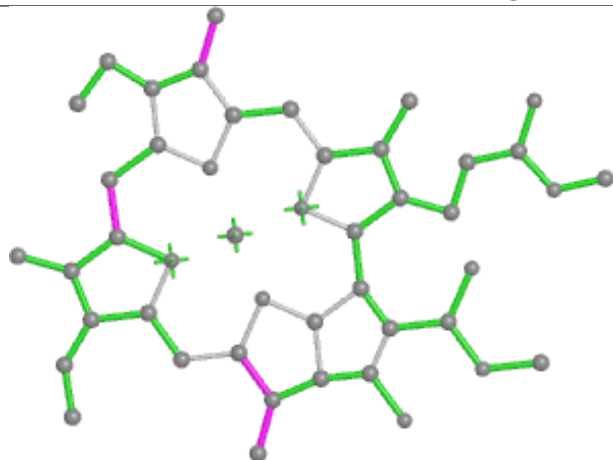
Rings

Ligand CLA A1 837

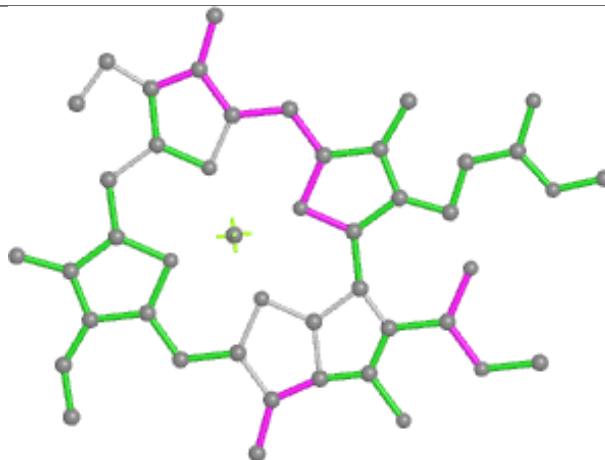




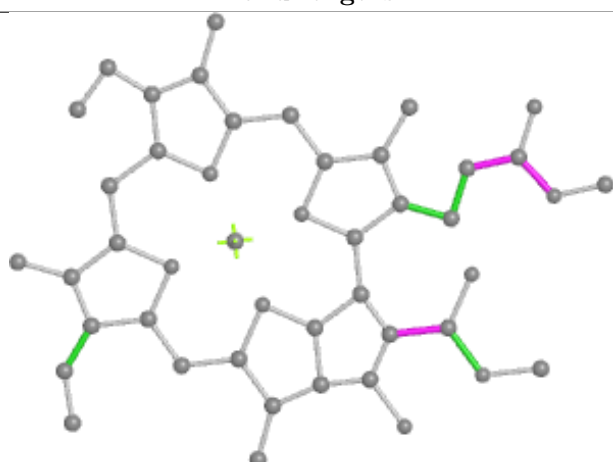
Ligand CLA A1 840



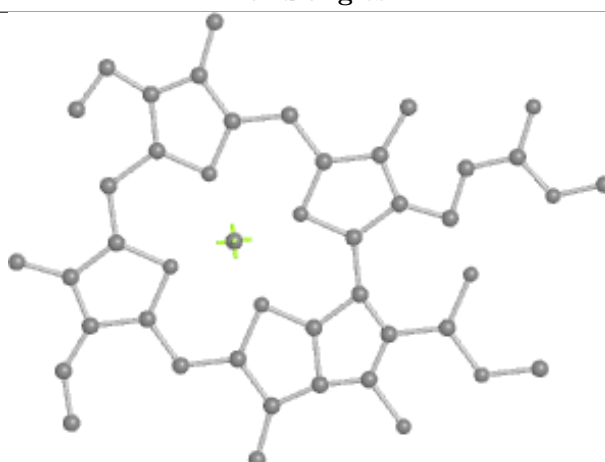
Bond lengths



Bond angles

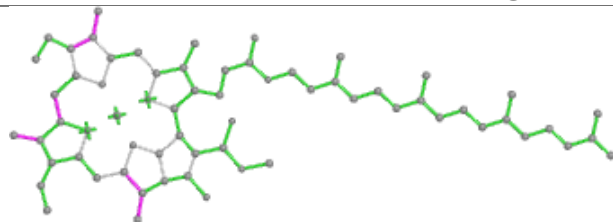


Torsions

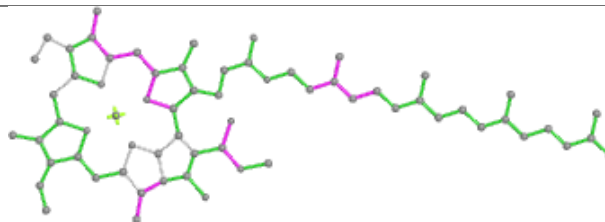


Rings

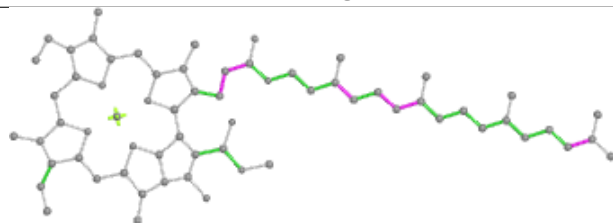
Ligand CLA A1 841



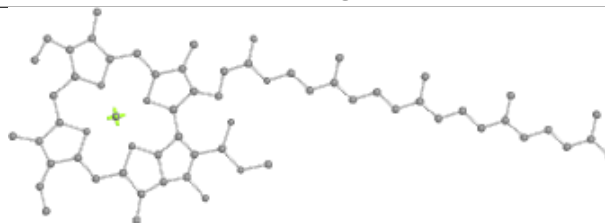
Bond lengths



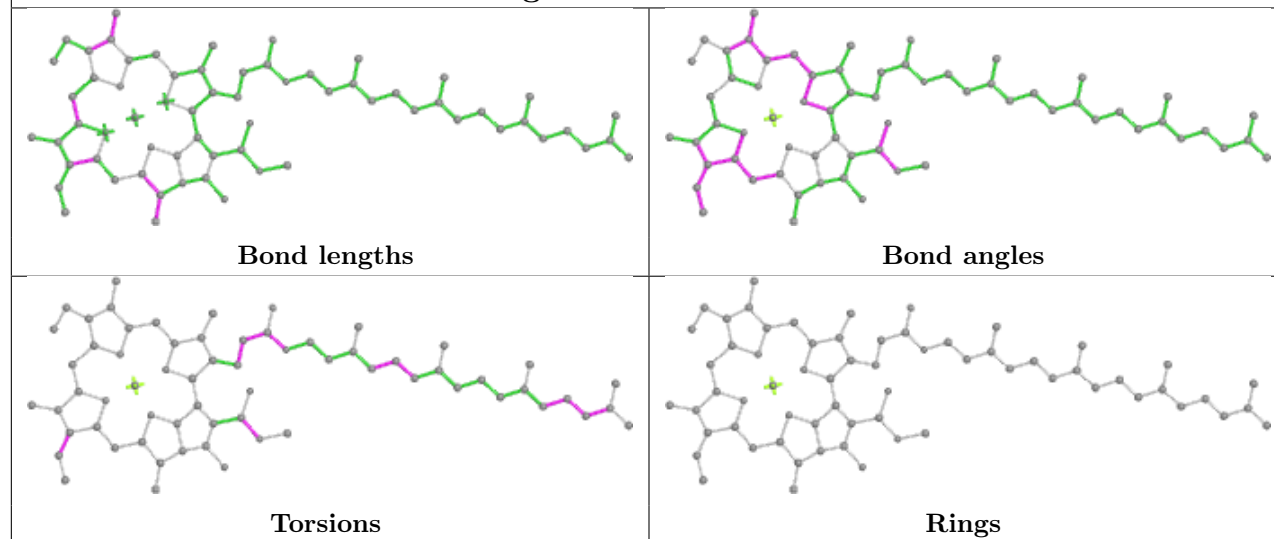
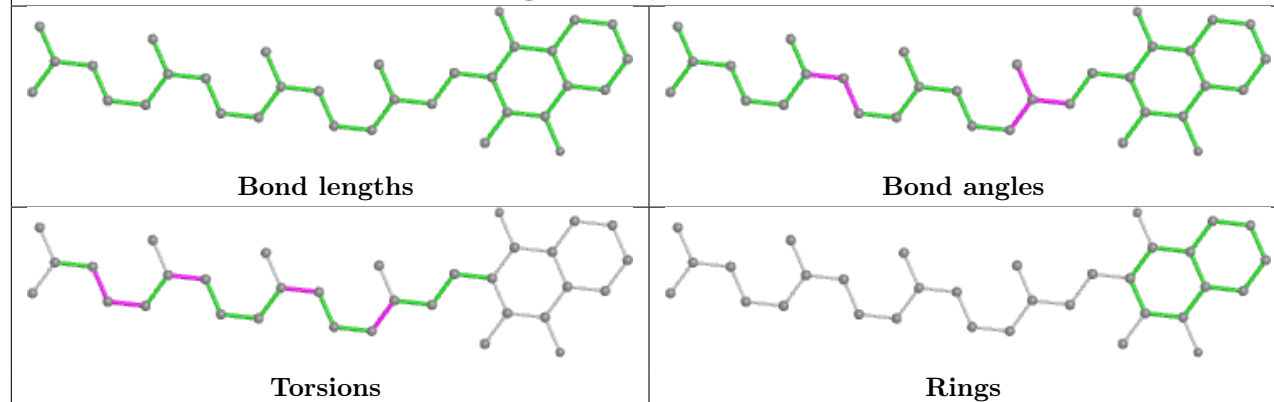
Bond angles



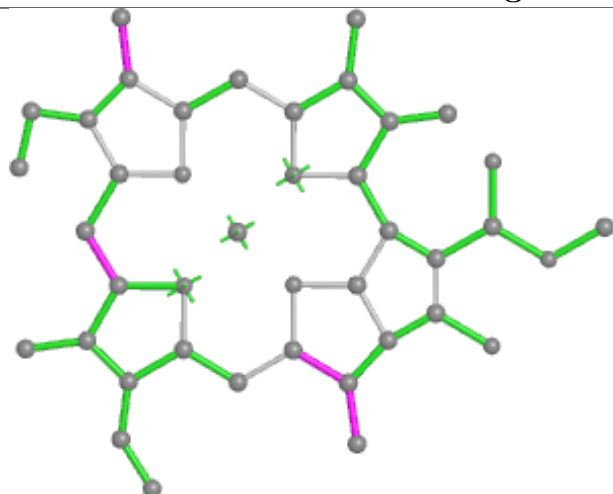
Torsions



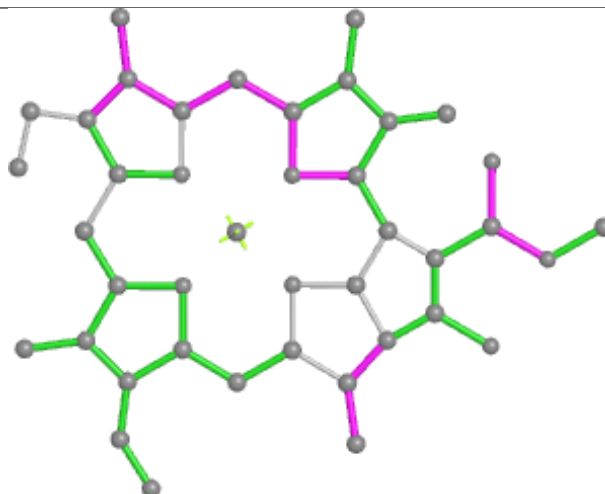
Rings

Ligand CLA A1 842**Ligand PQN A1 843**

Ligand CLA A1 844



Bond lengths



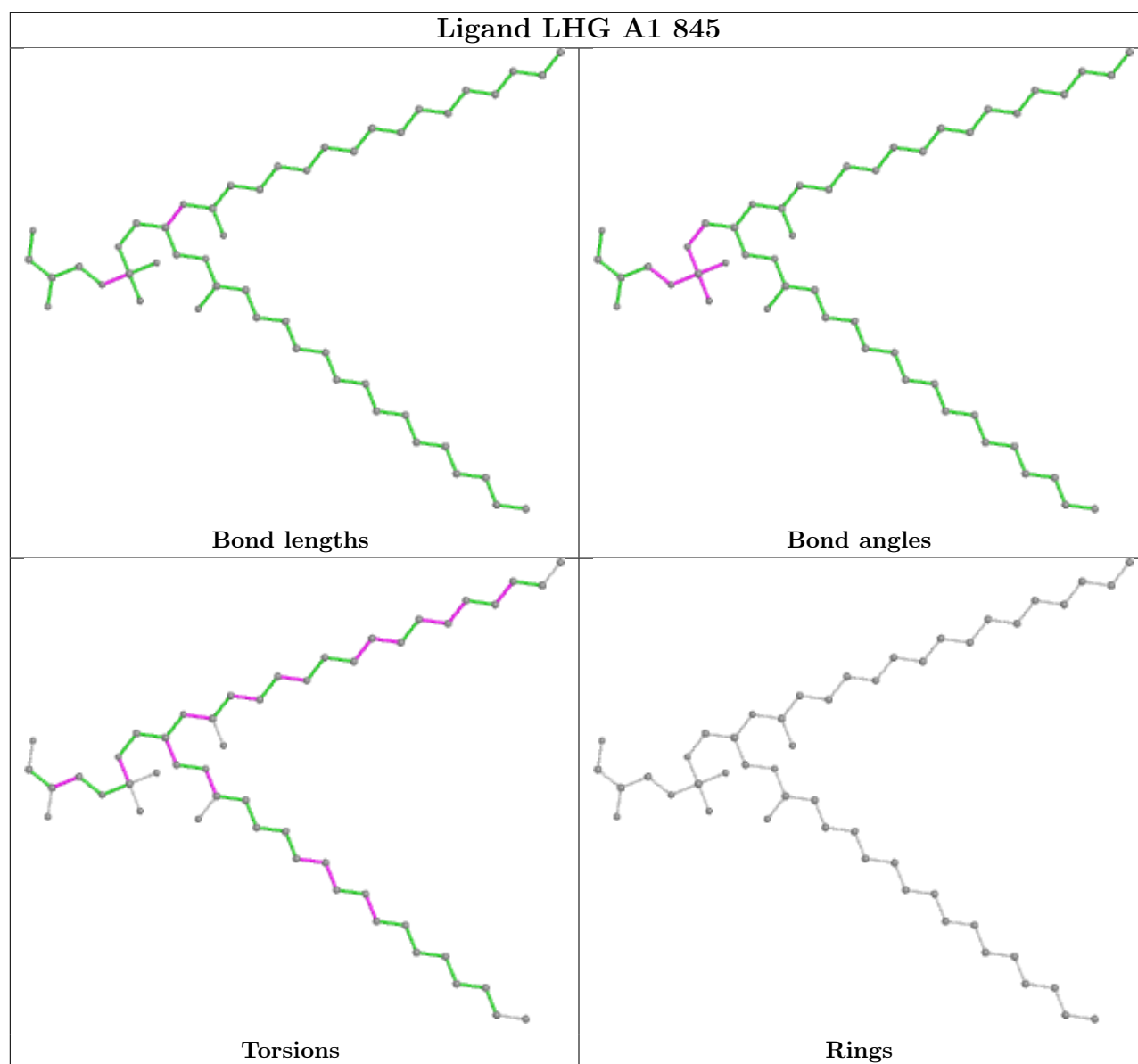
Bond angles

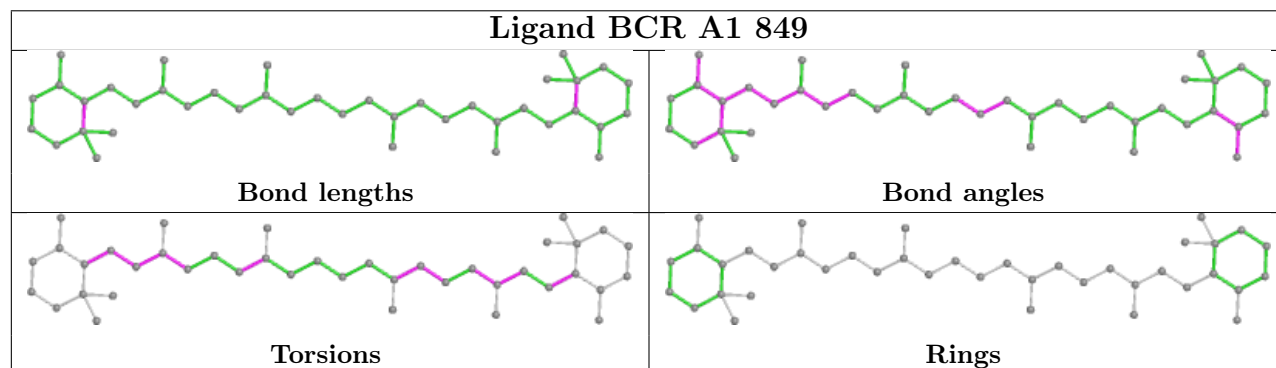
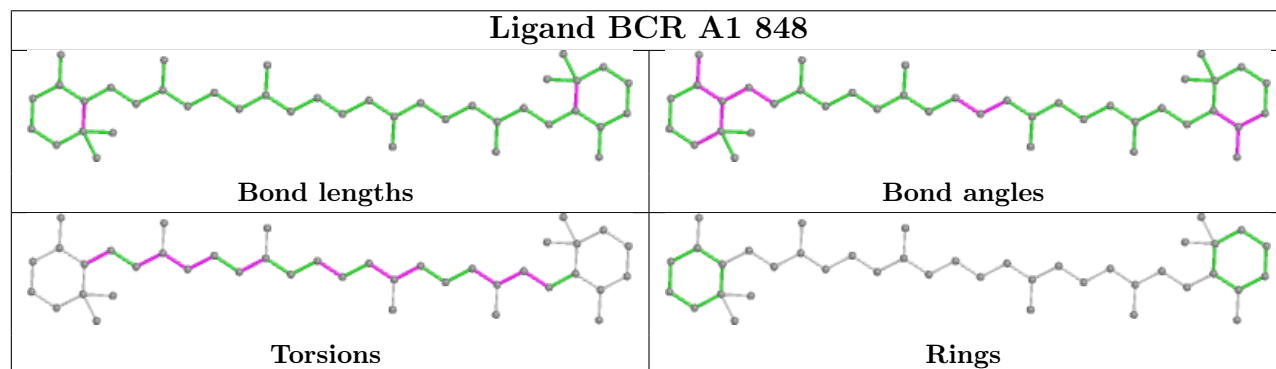
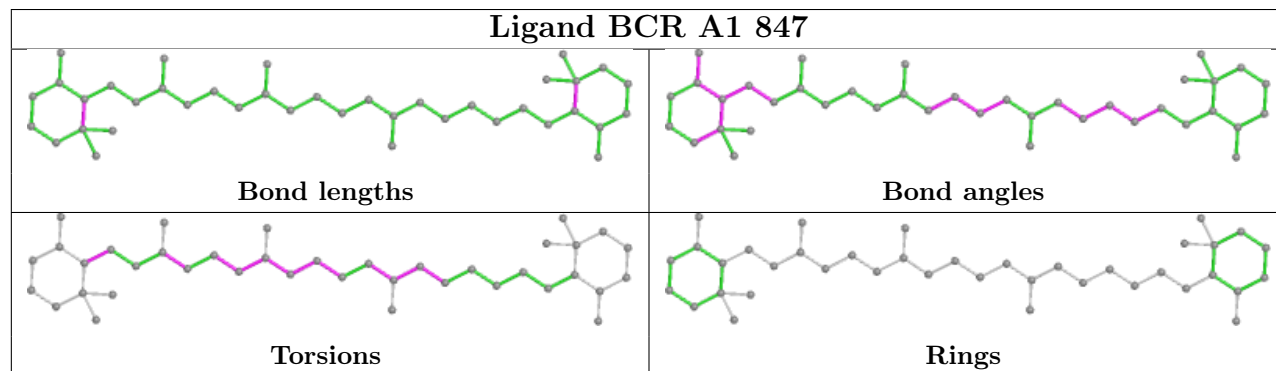
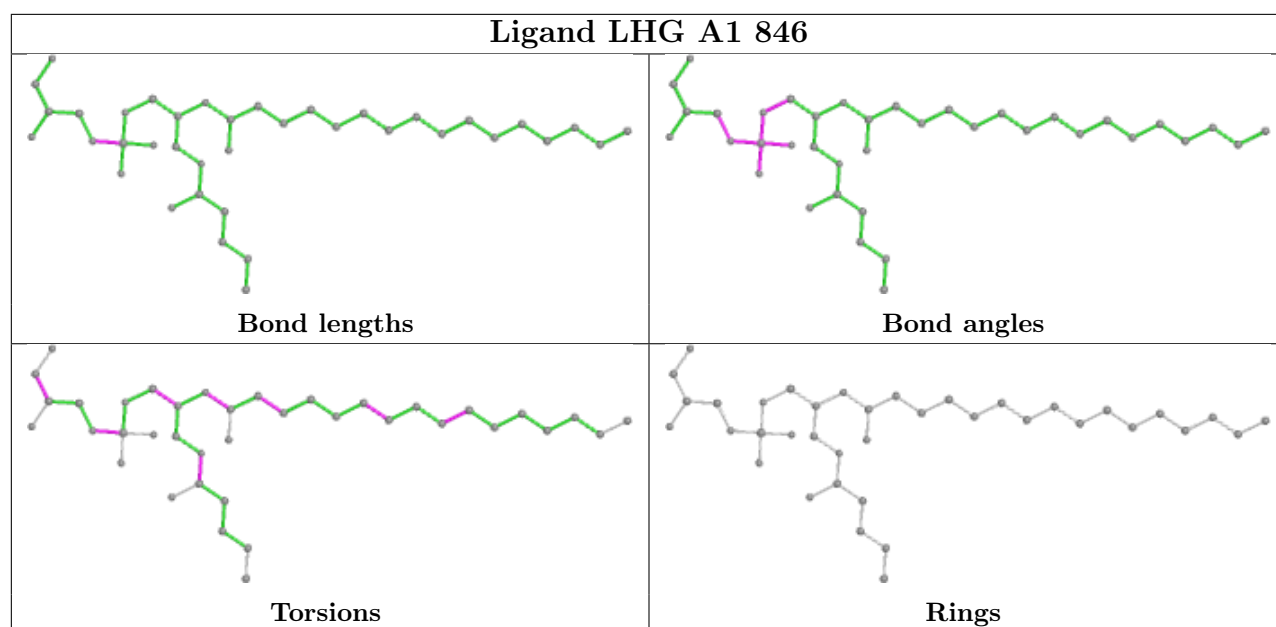


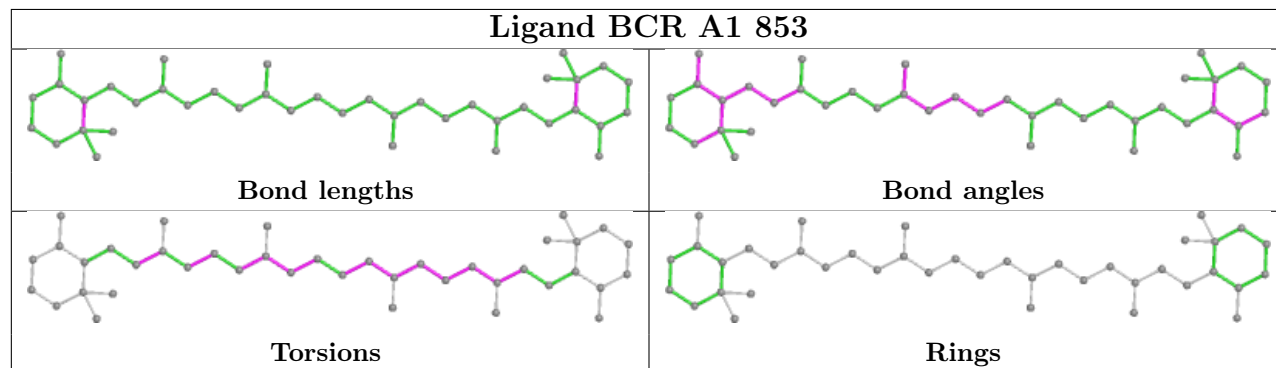
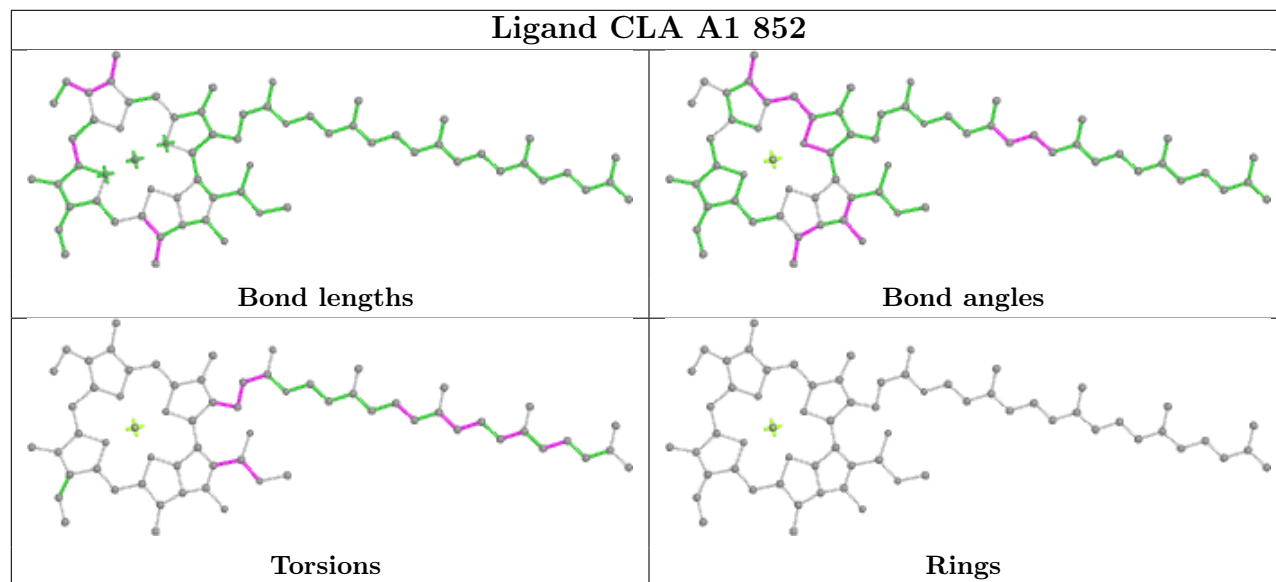
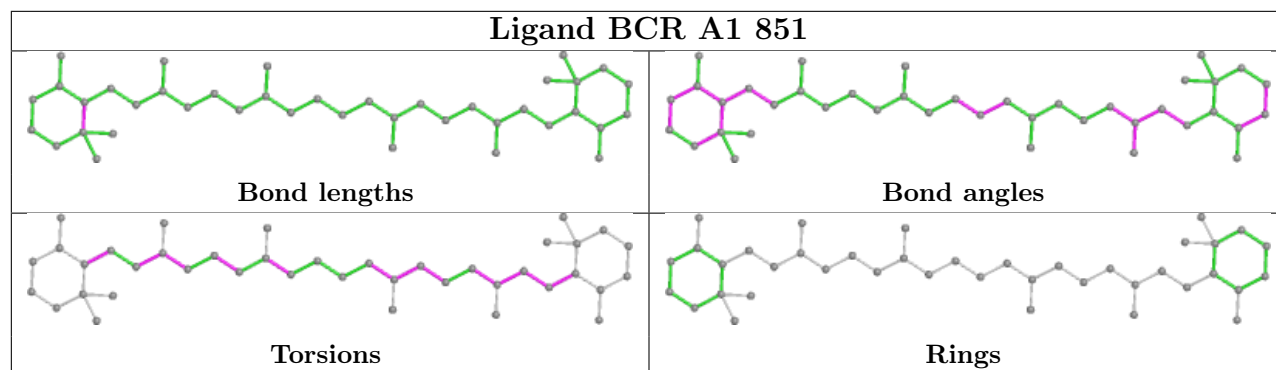
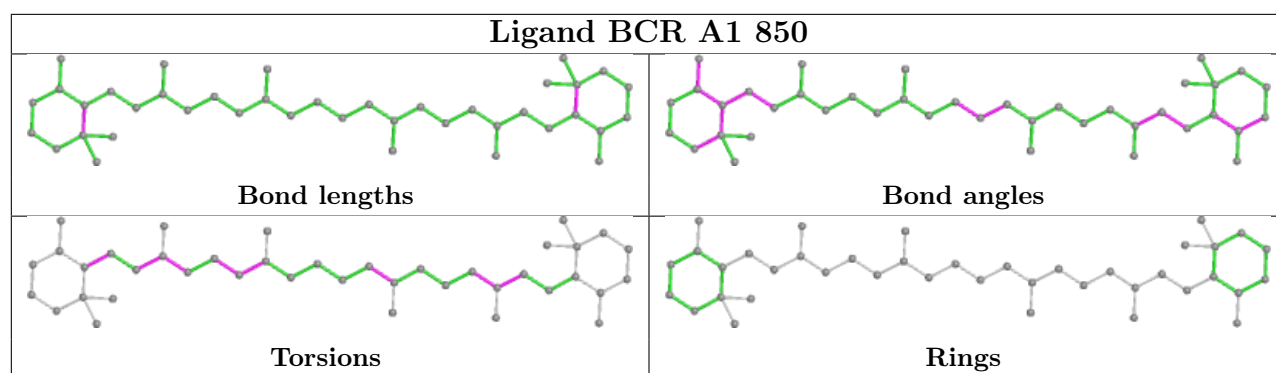
Torsions

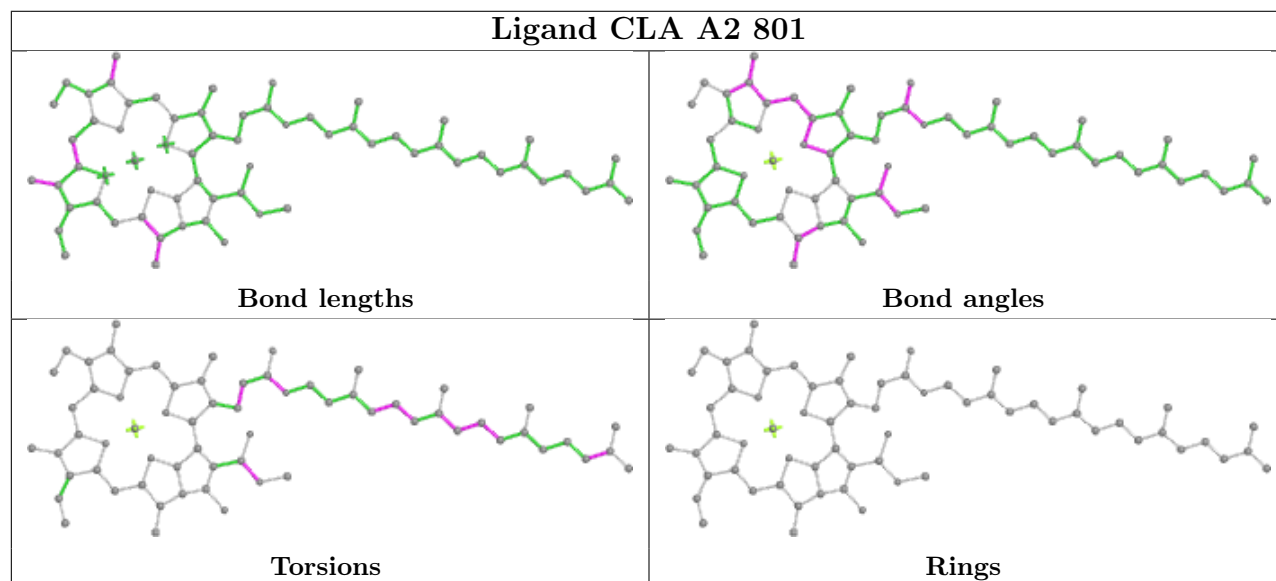
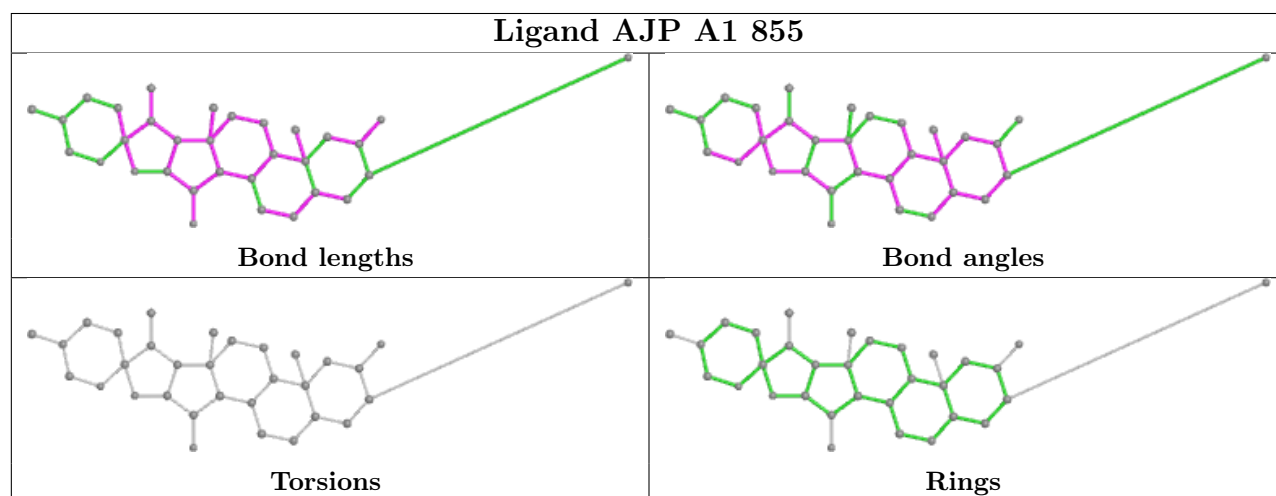
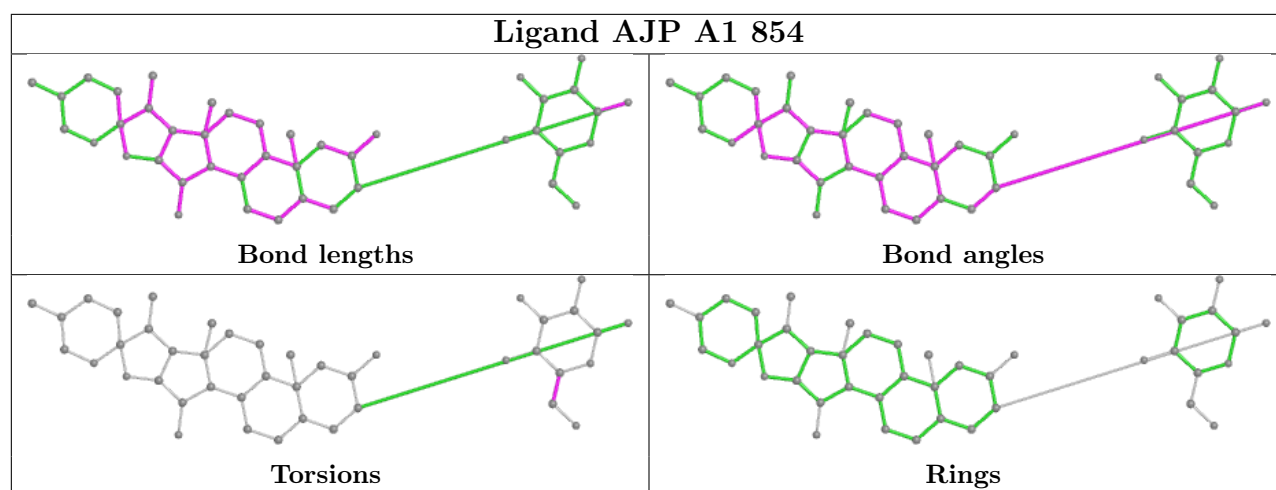


Rings

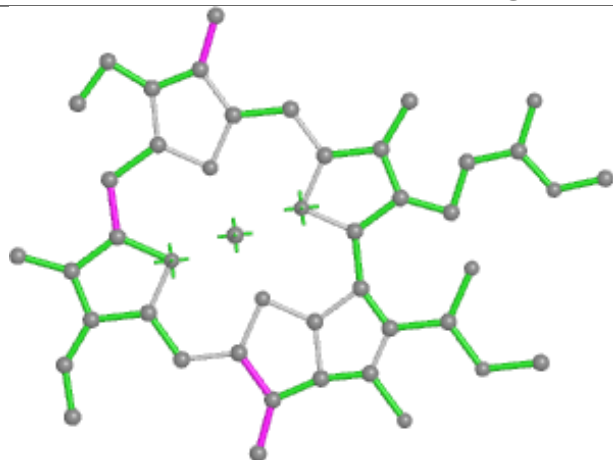




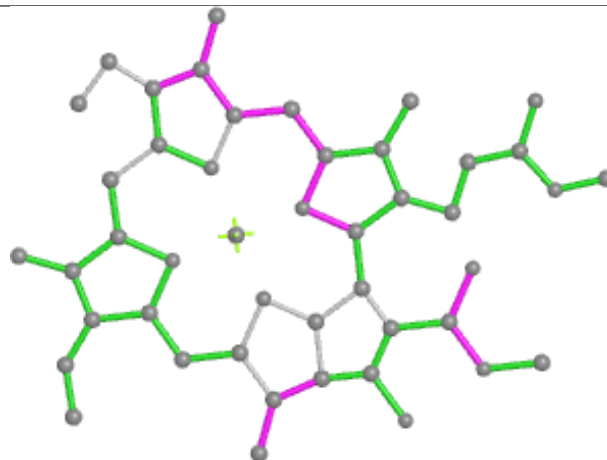




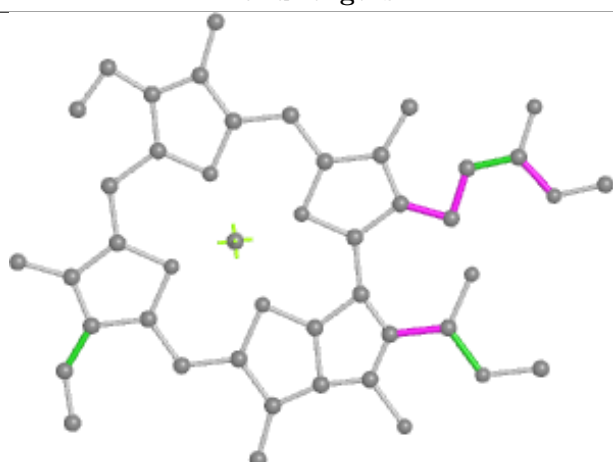
Ligand CLA A2 802



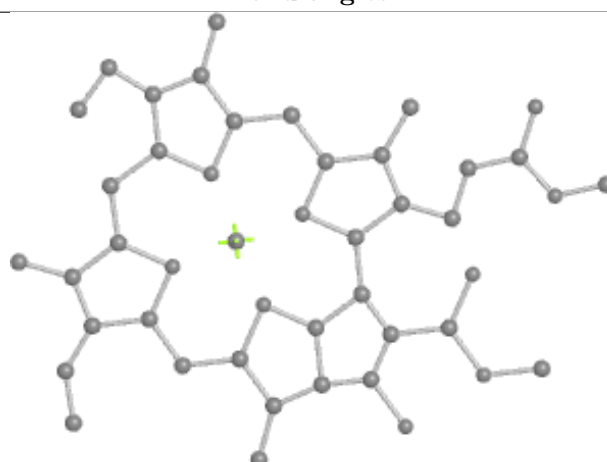
Bond lengths



Bond angles

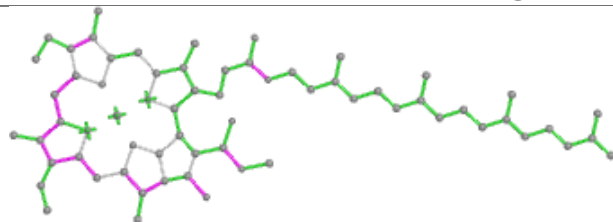


Torsions

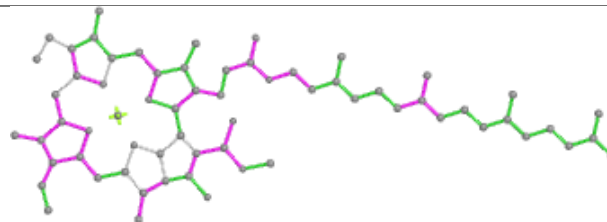


Rings

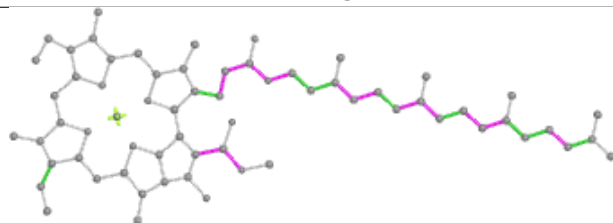
Ligand CL0 A2 803



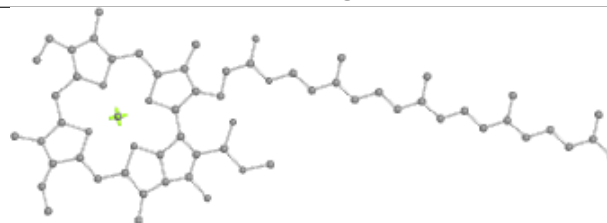
Bond lengths



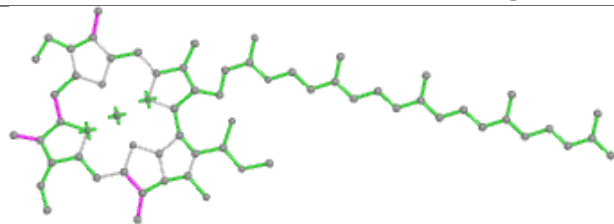
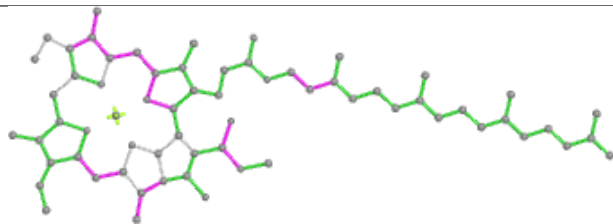
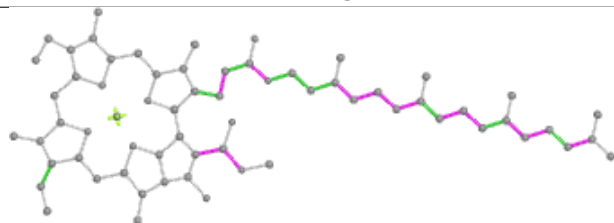
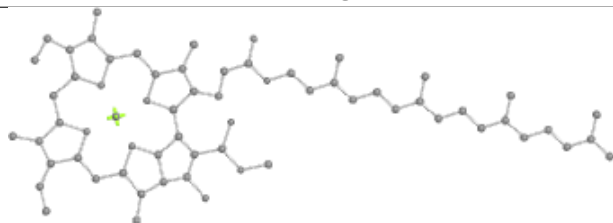
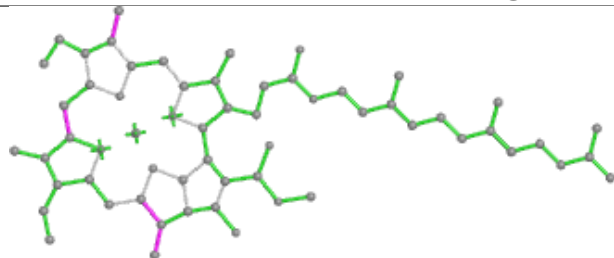
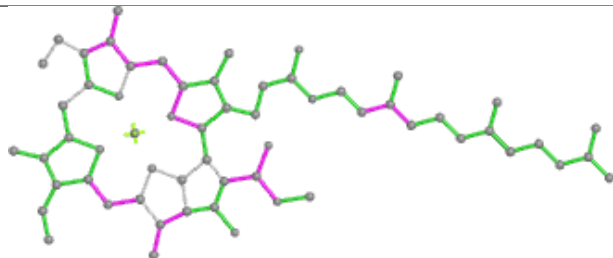
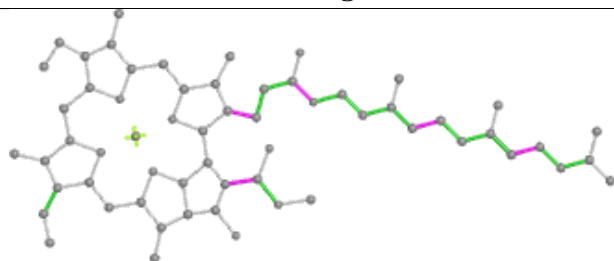
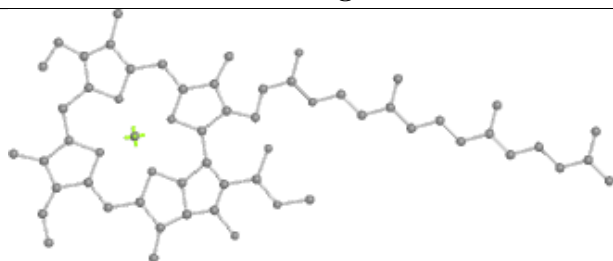
Bond angles



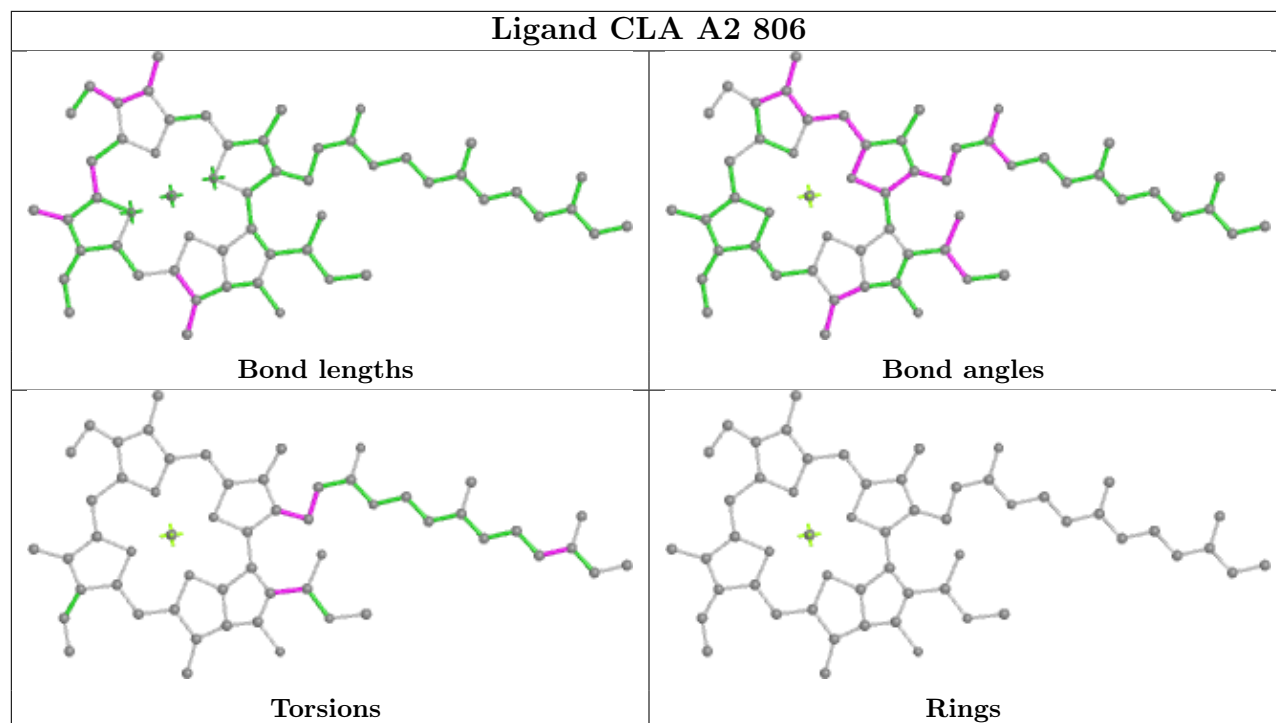
Torsions



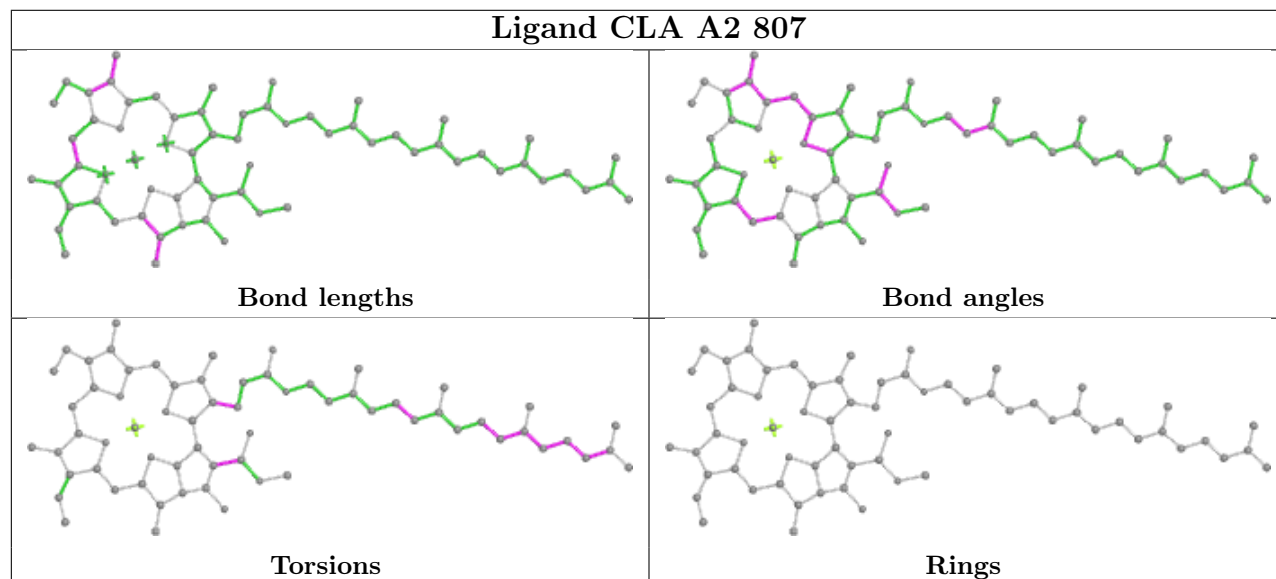
Rings

Ligand CLA A2 804**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A2 805****Bond lengths****Bond angles****Torsions****Rings**

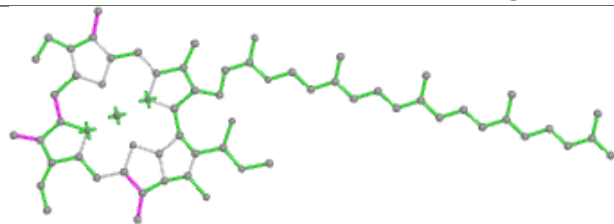
Ligand CLA A2 806



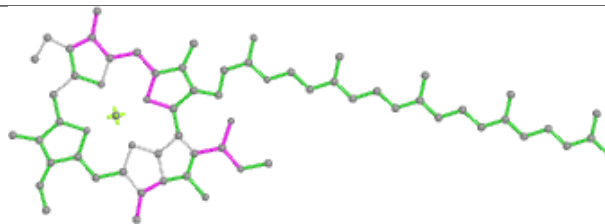
Ligand CLA A2 807



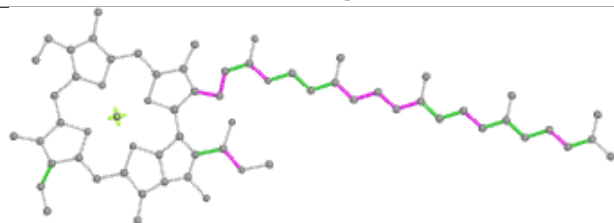
Ligand CLA A2 808



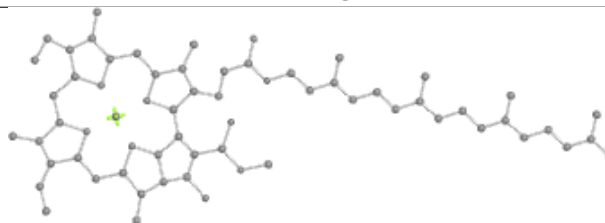
Bond lengths



Bond angles

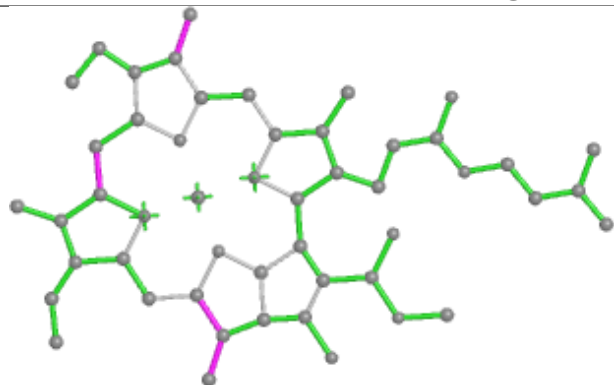


Torsions

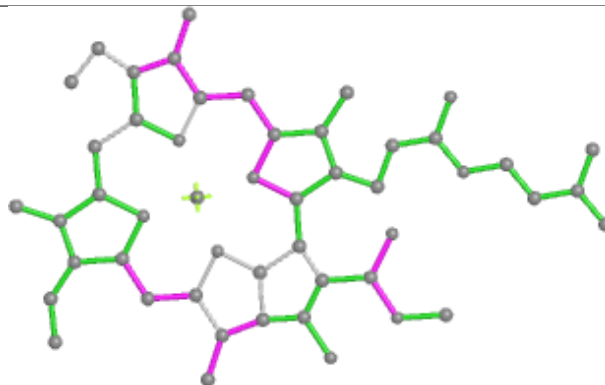


Rings

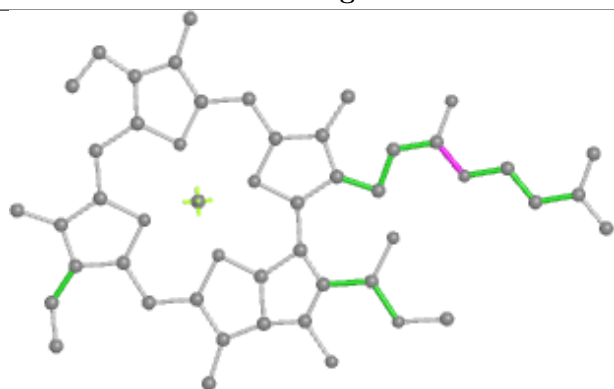
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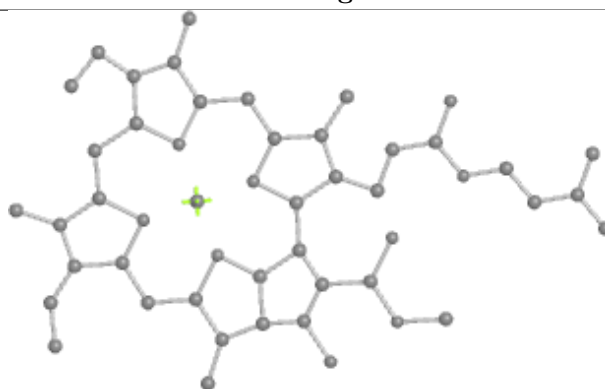
Bond lengths



Bond angles

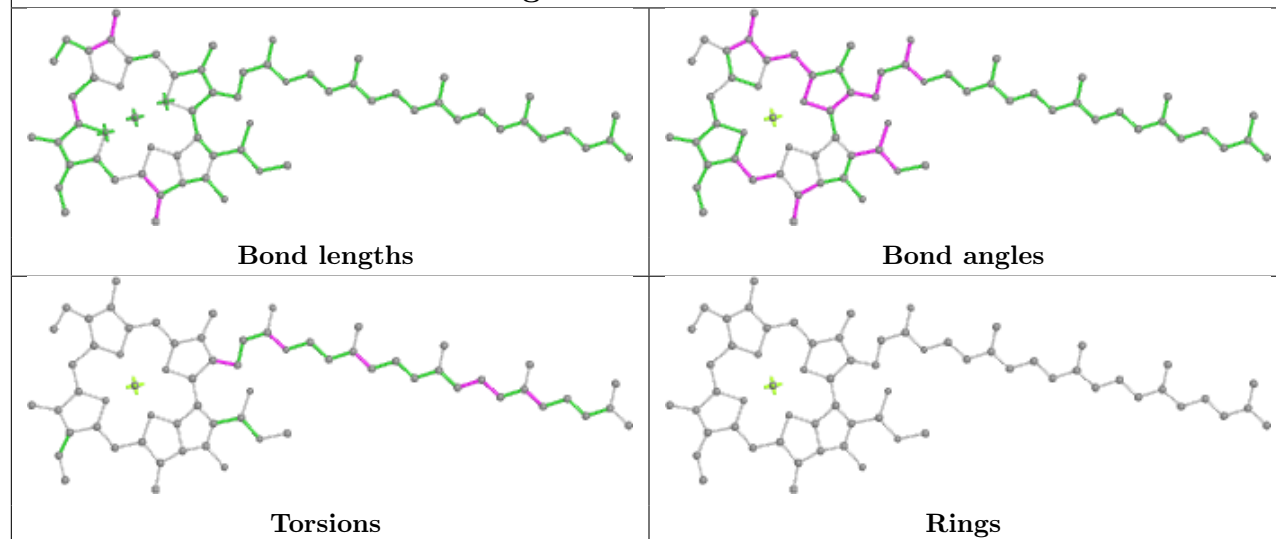


Torsions

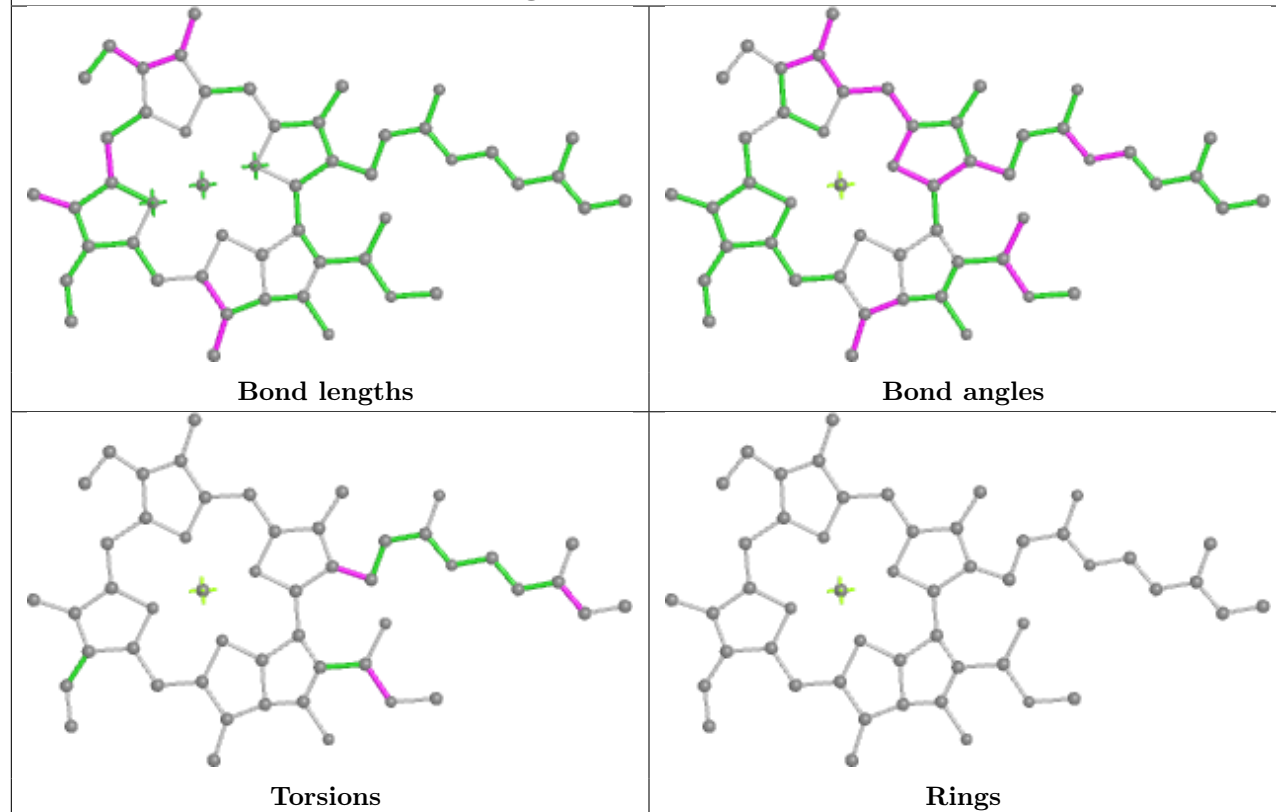


Rings

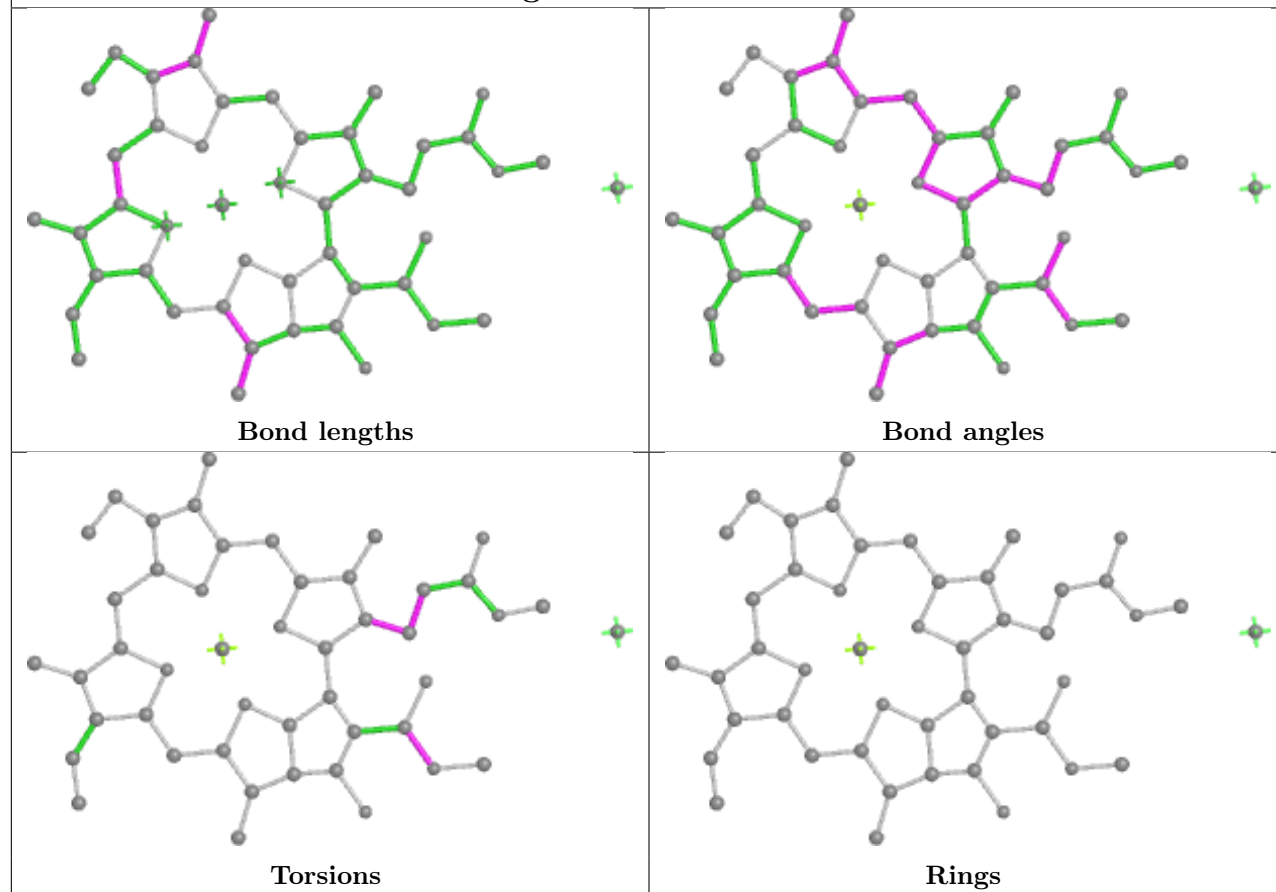
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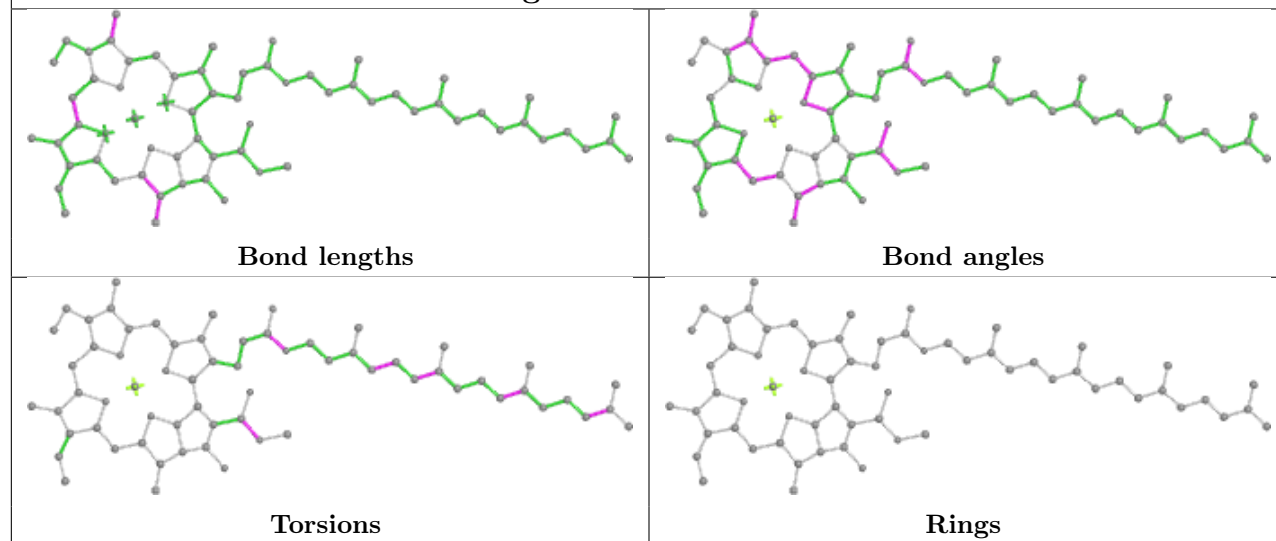
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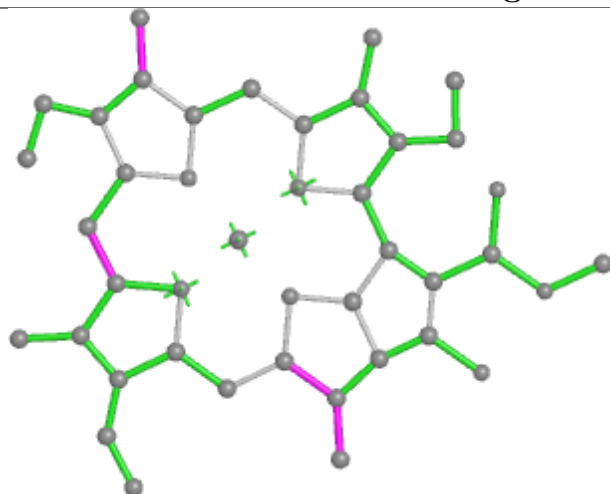
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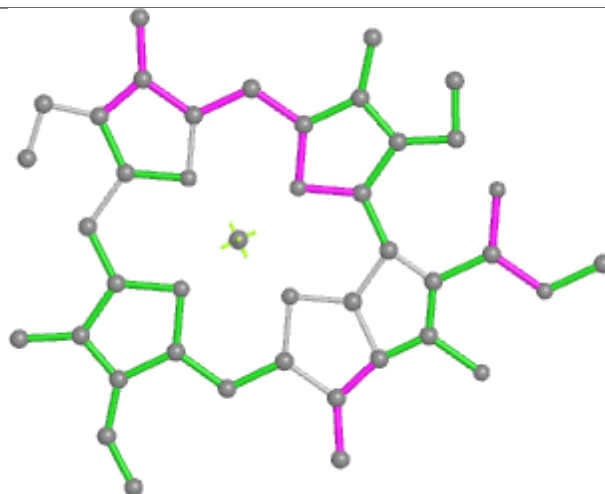
Ligand CLA A2 813



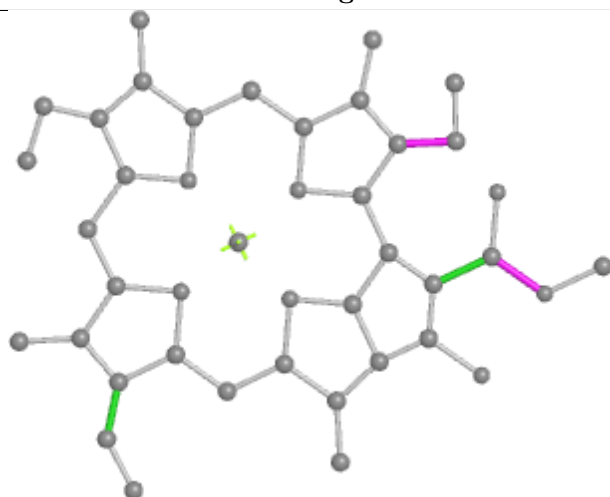
Ligand CLA A2 814



Bond lengths



Bond angles

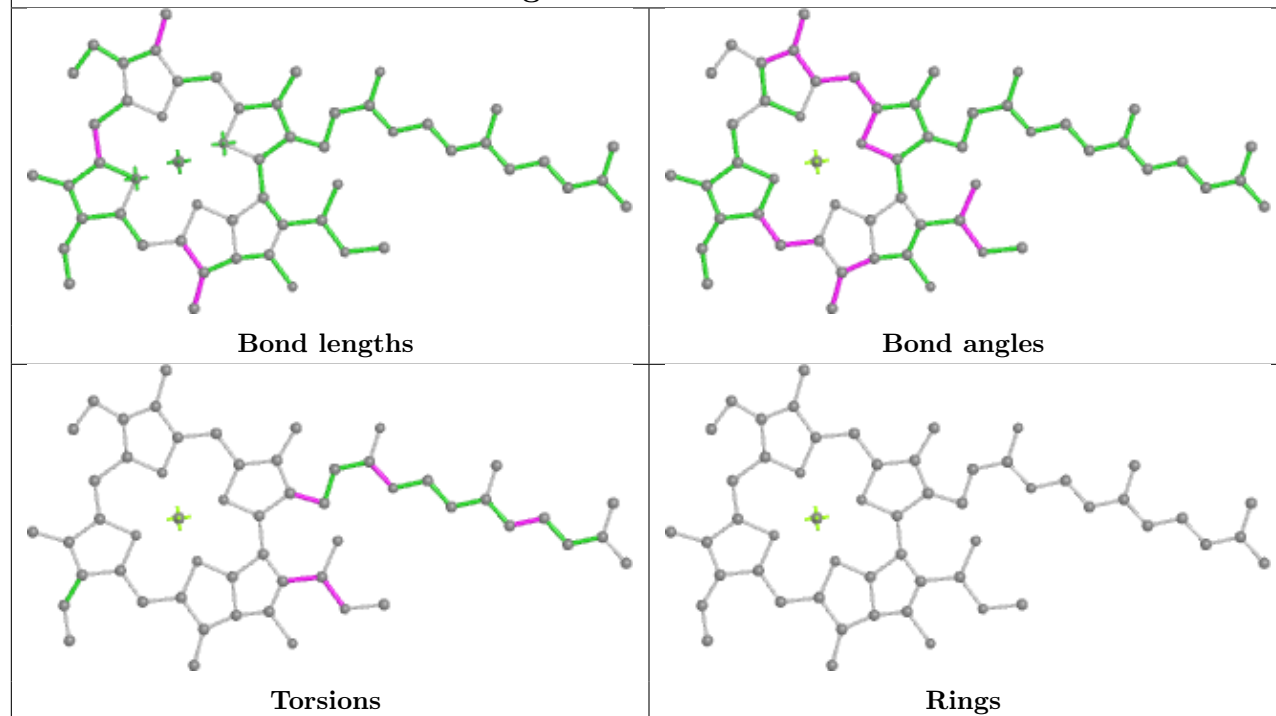


Torsions

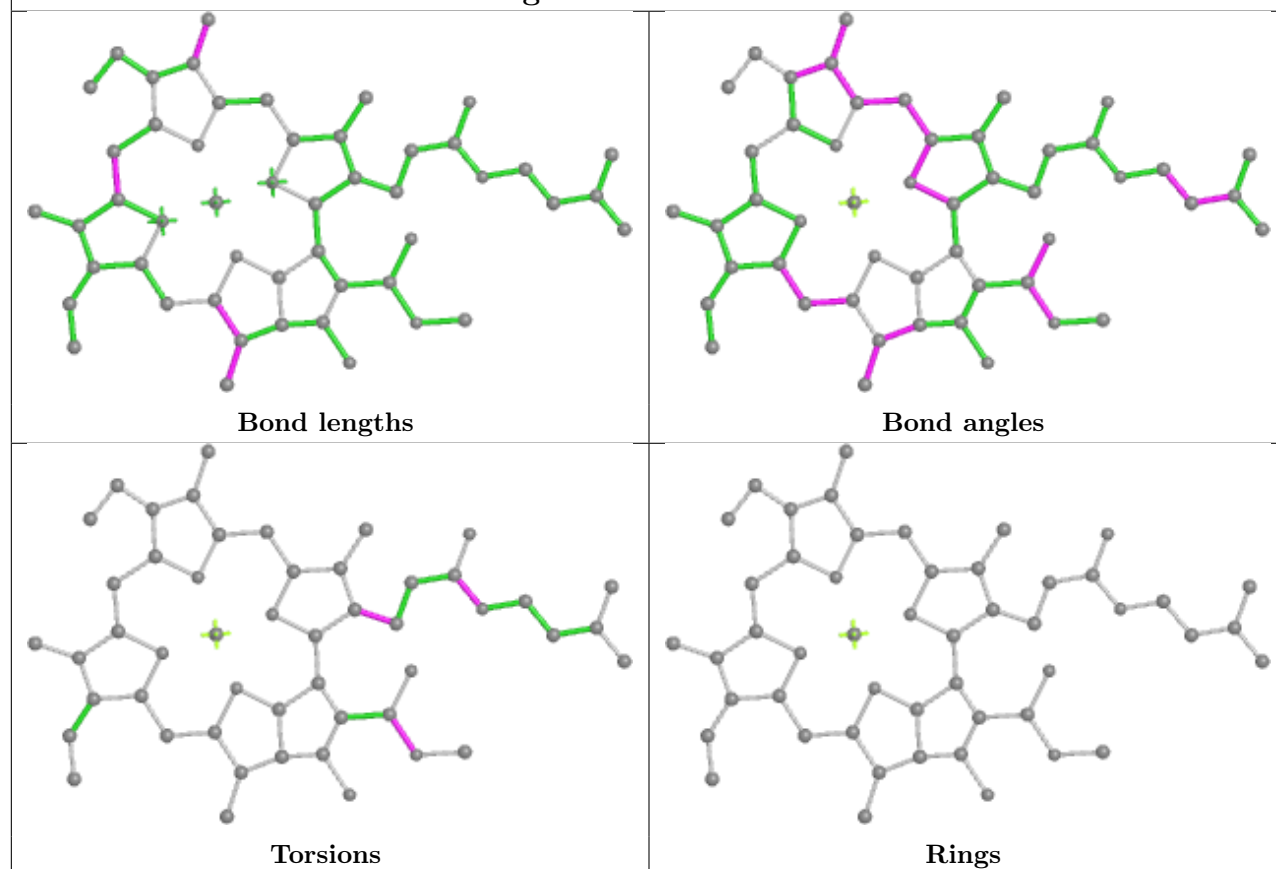


Rings

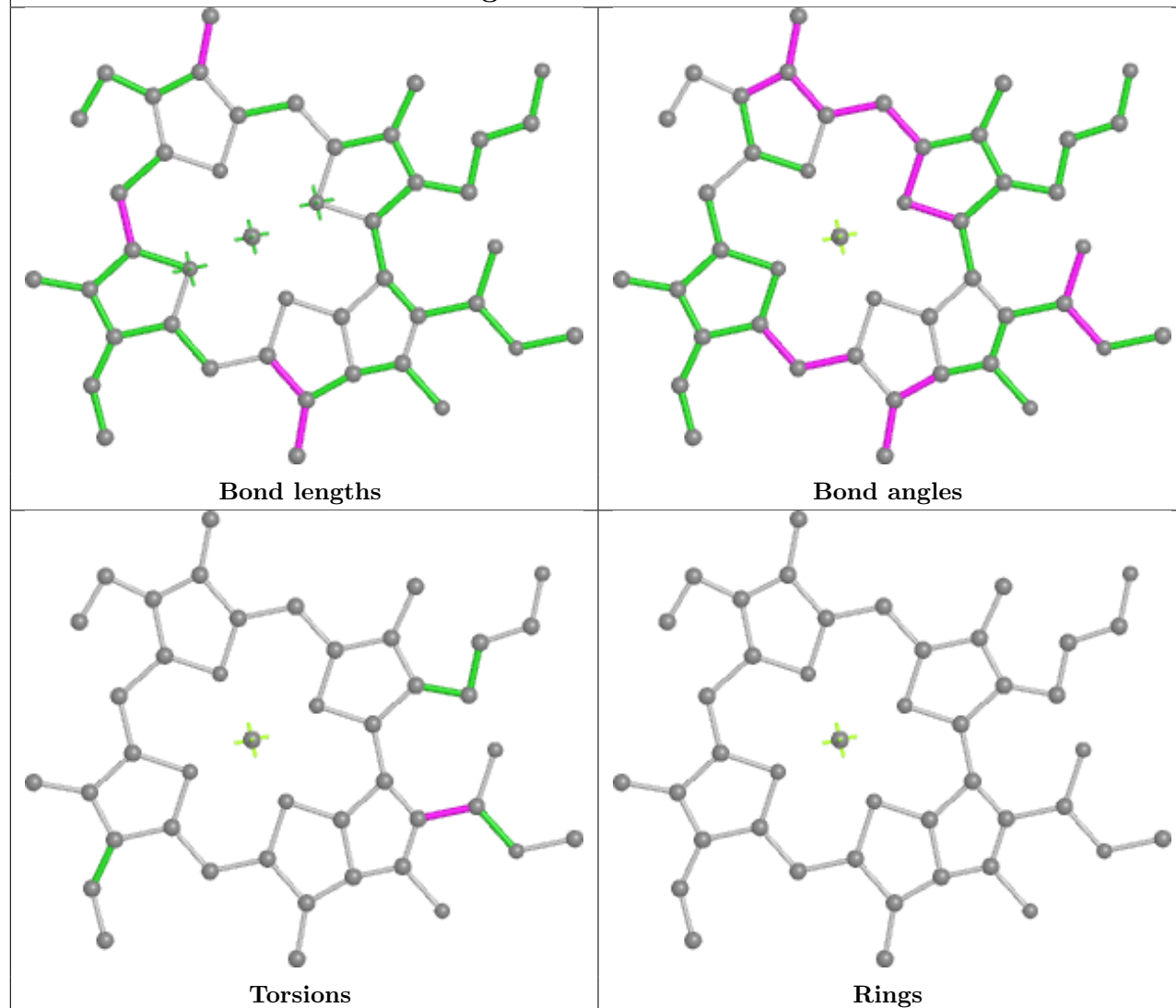
Ligand CLA A2 815



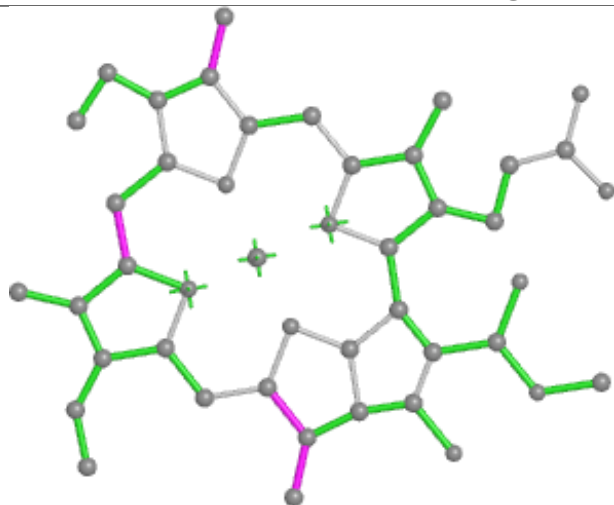
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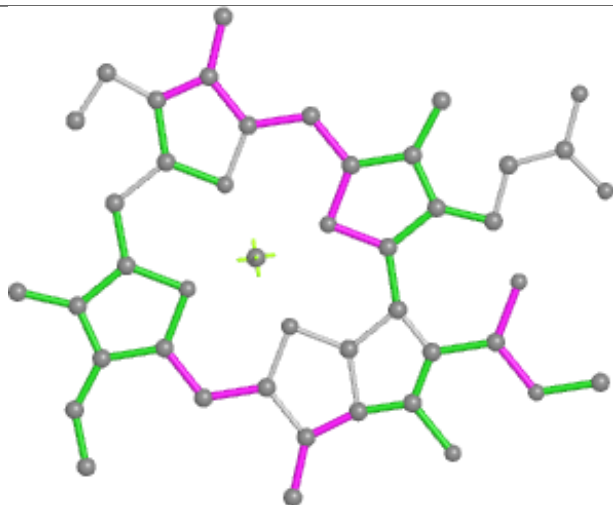
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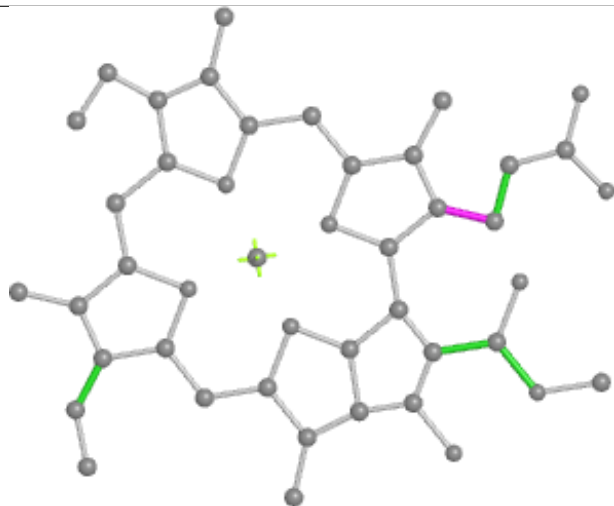
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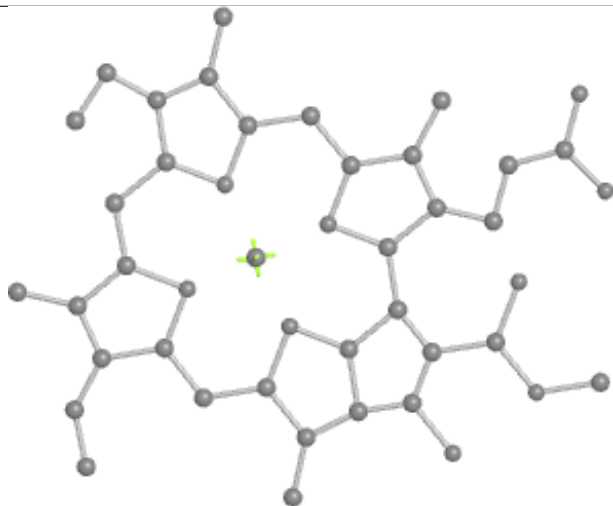
Bond lengths



Bond angles

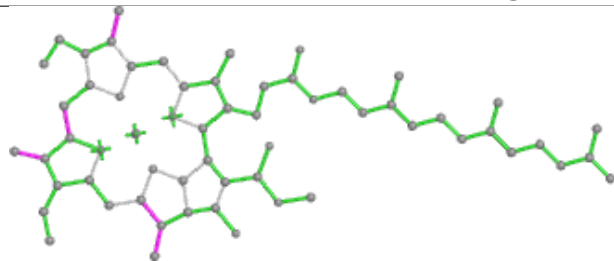


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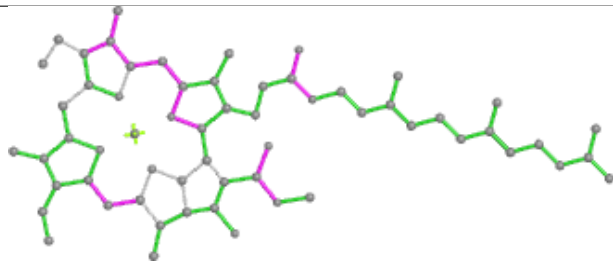


Rings

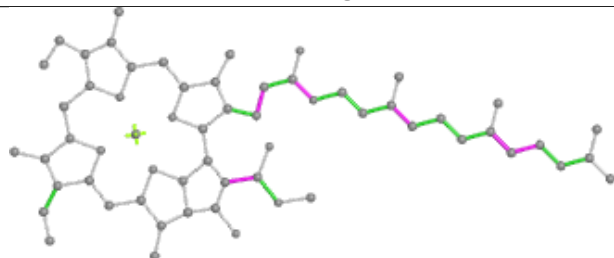
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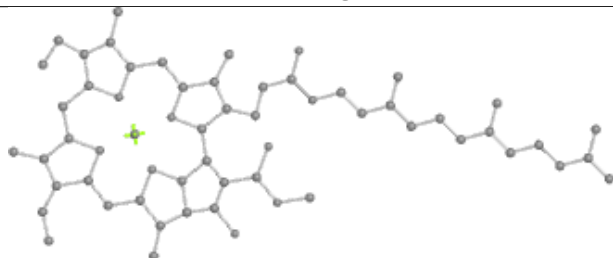
Bond lengths



Bond angles

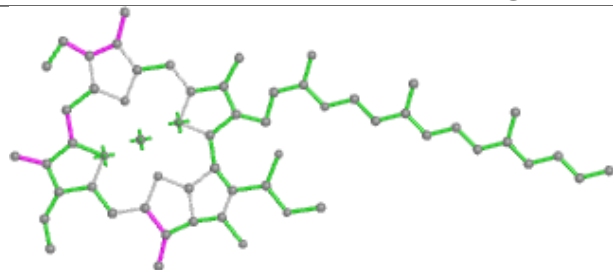


Torsions

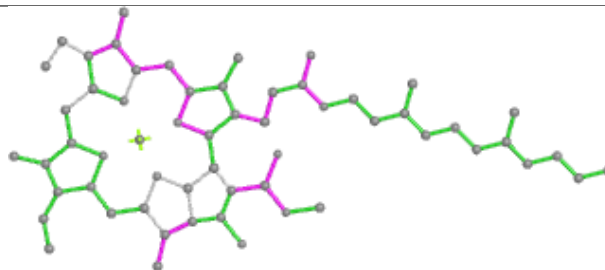


Rings

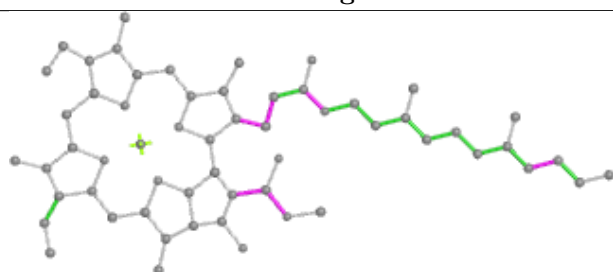
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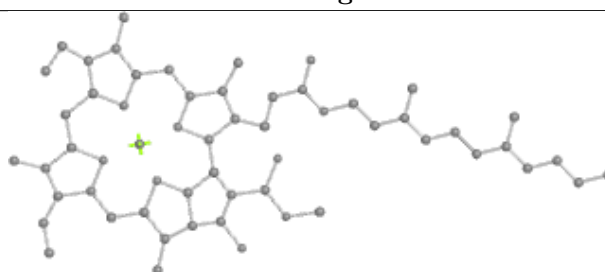
Bond lengths



Bond angles

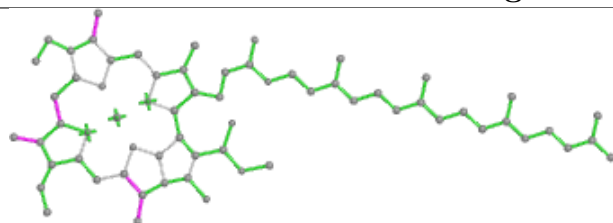


Torsions

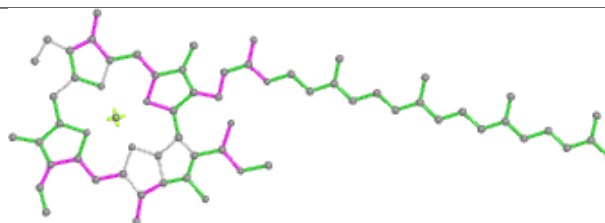


Rings

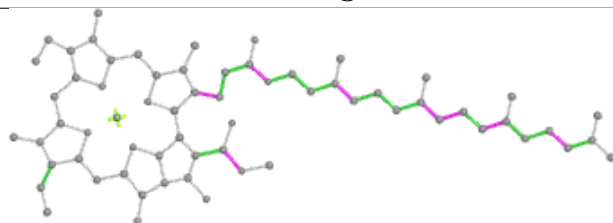
Ligand CLA A2 821



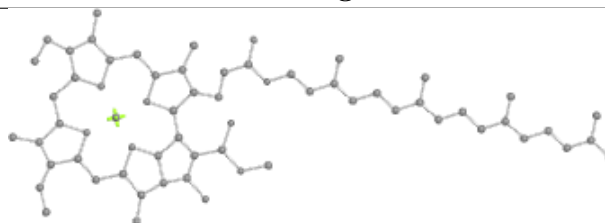
Bond lengths



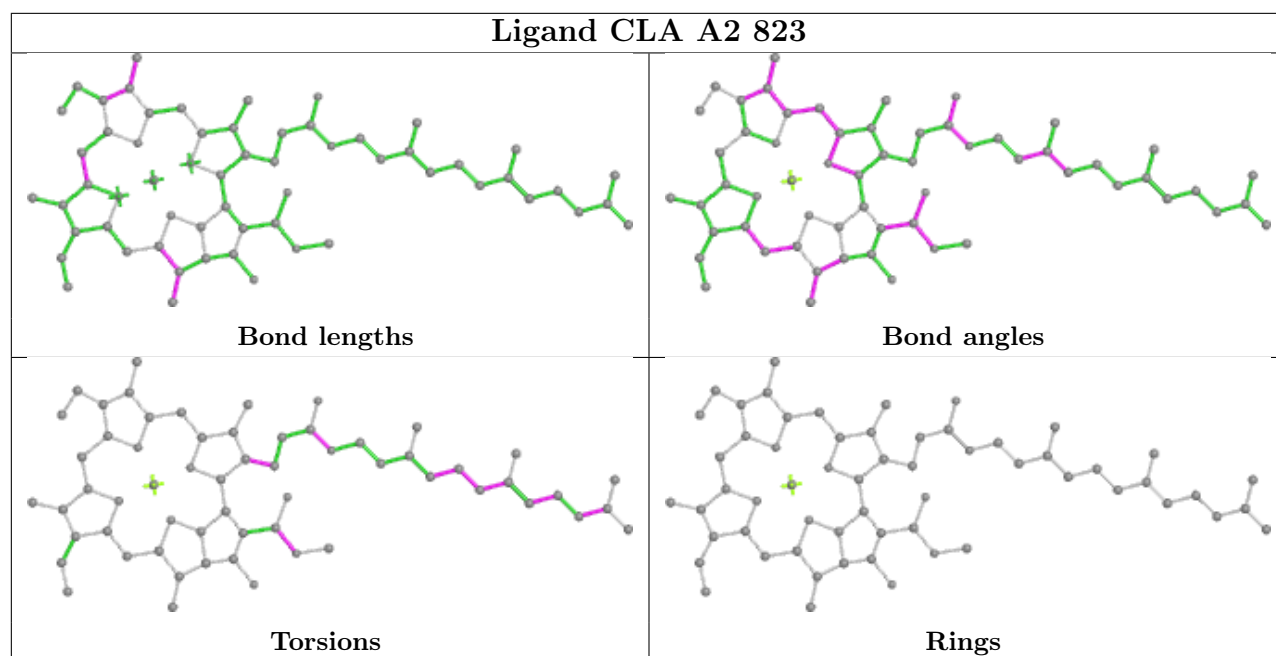
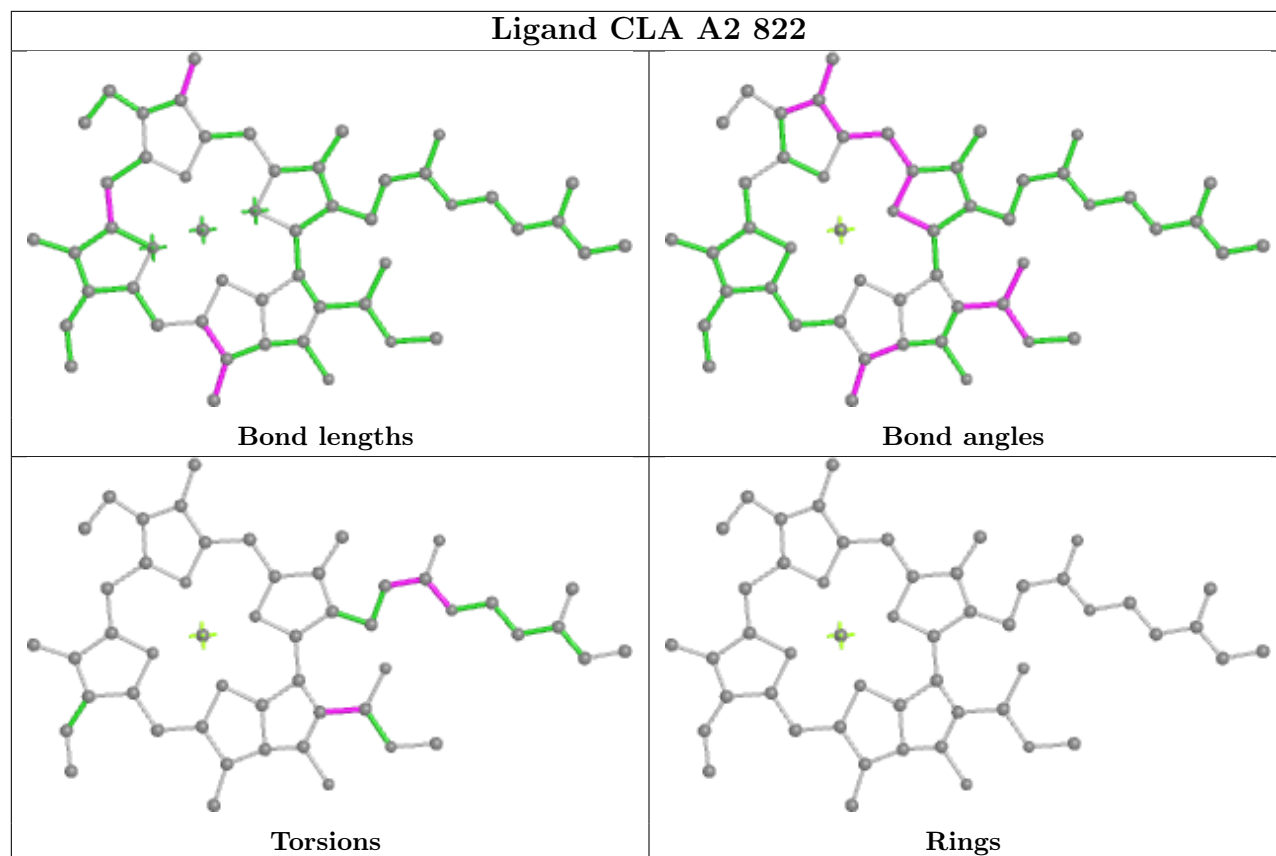
Bond angles



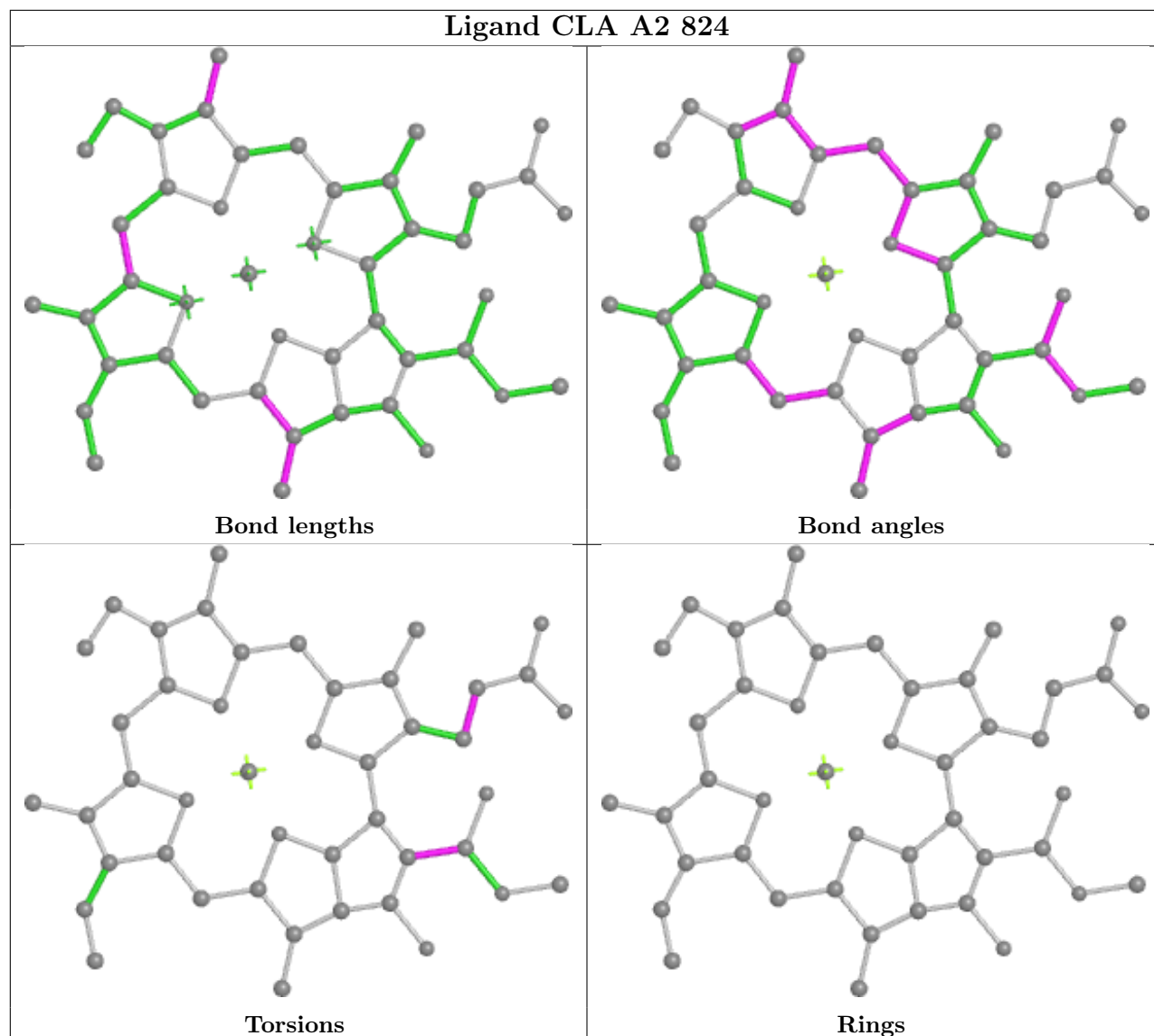
Torsions



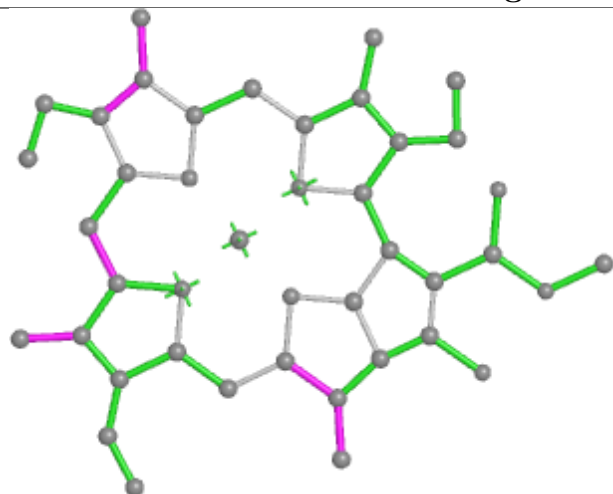
Rings



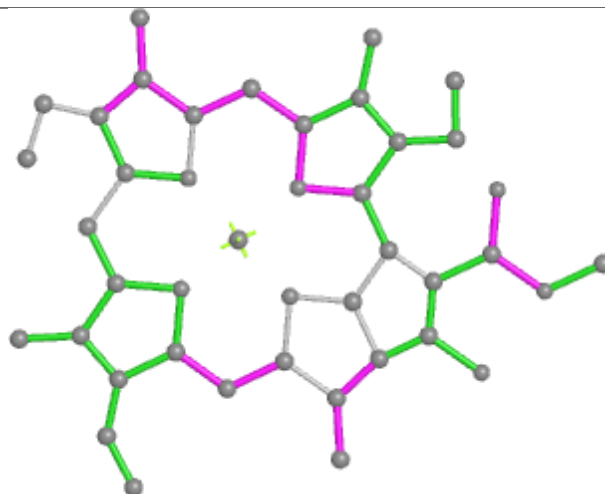
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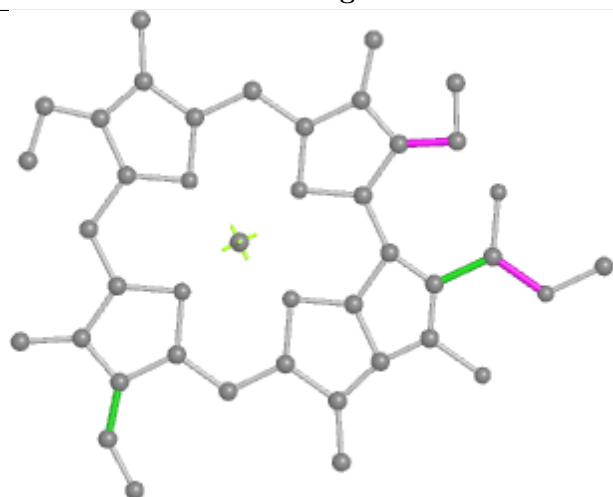
Ligand CLA A2 825



Bond lengths



Bond angles

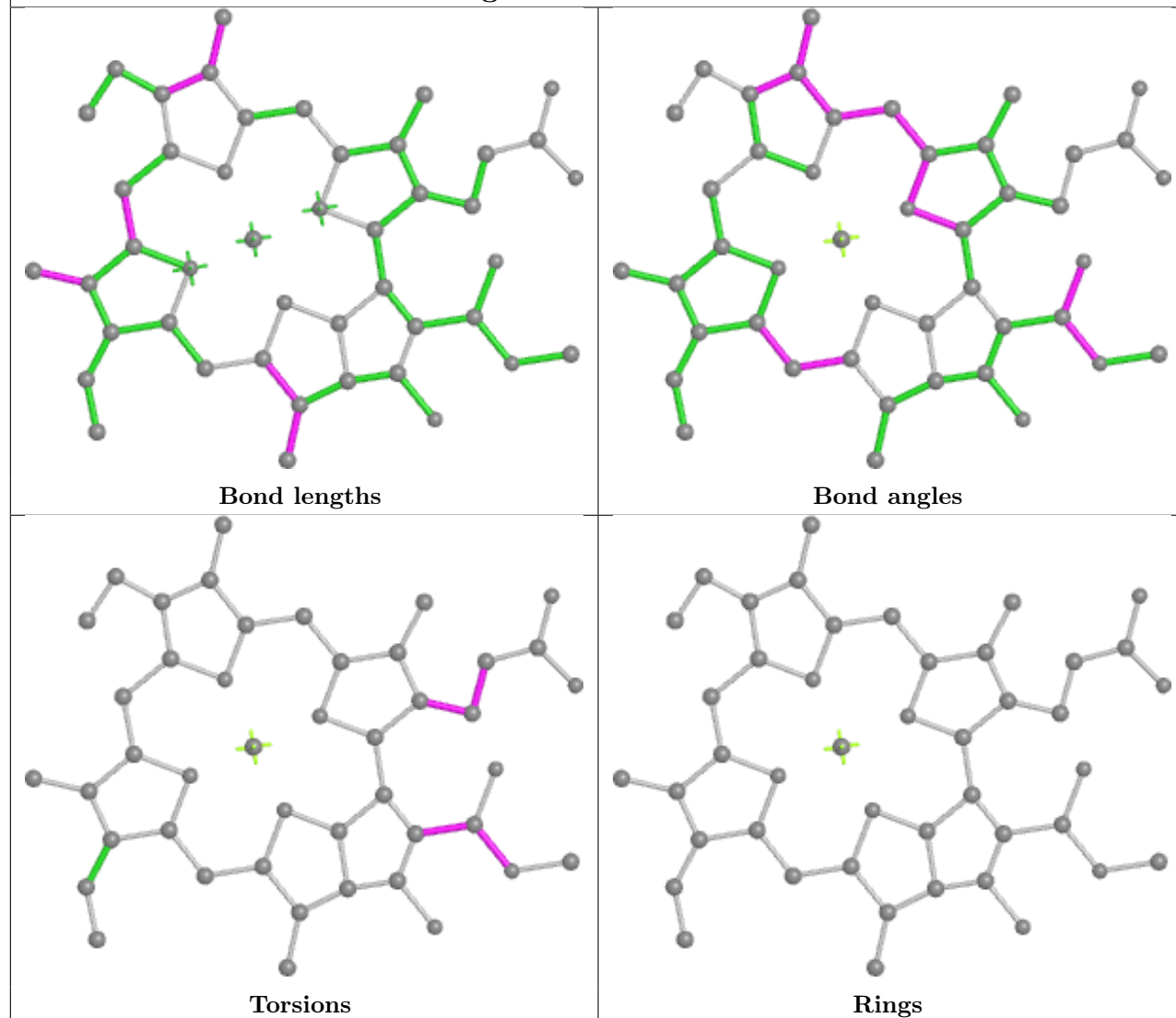


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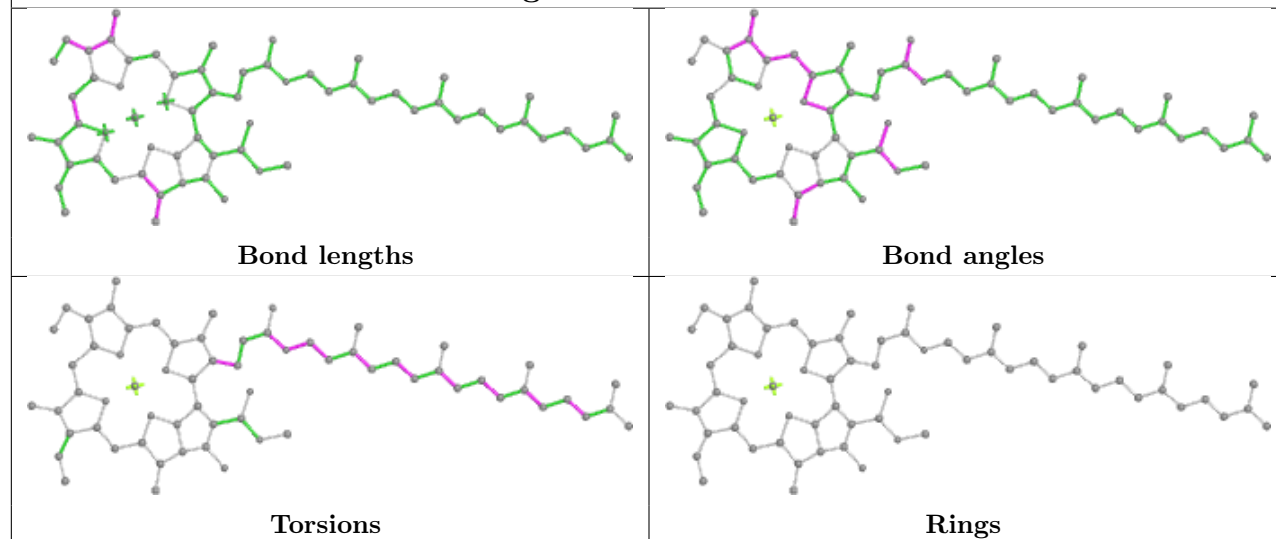


Rings

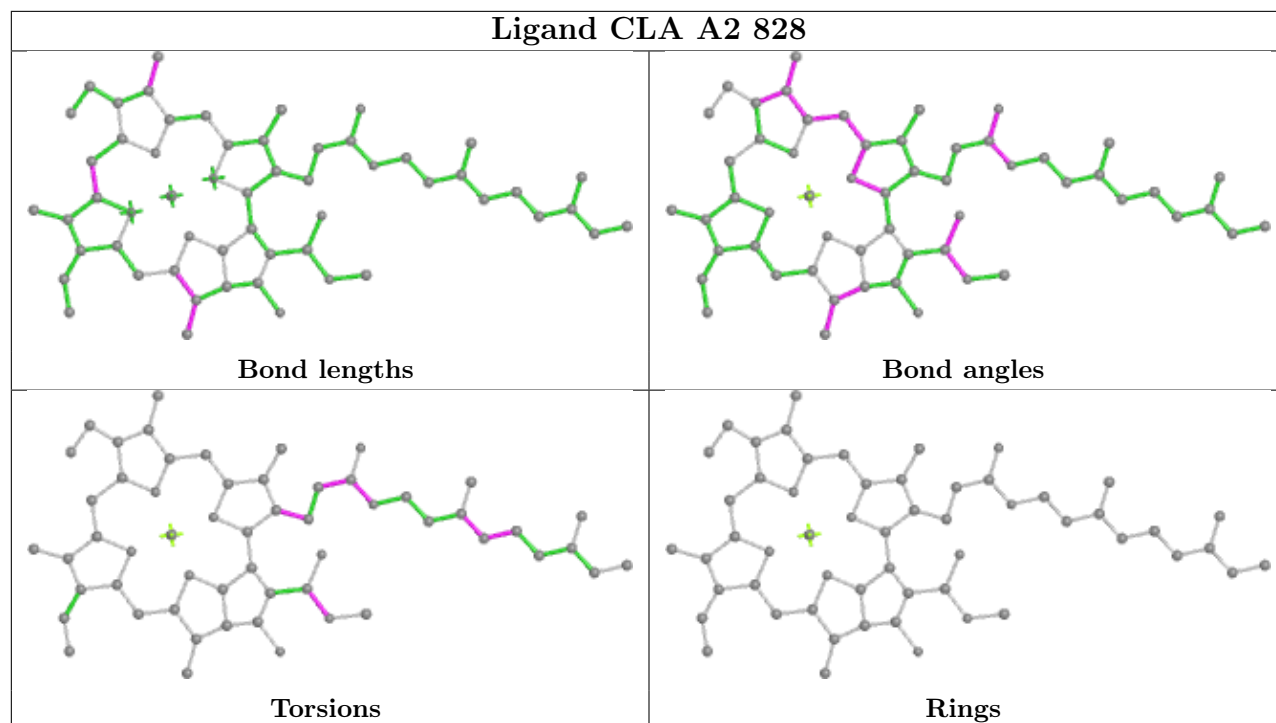
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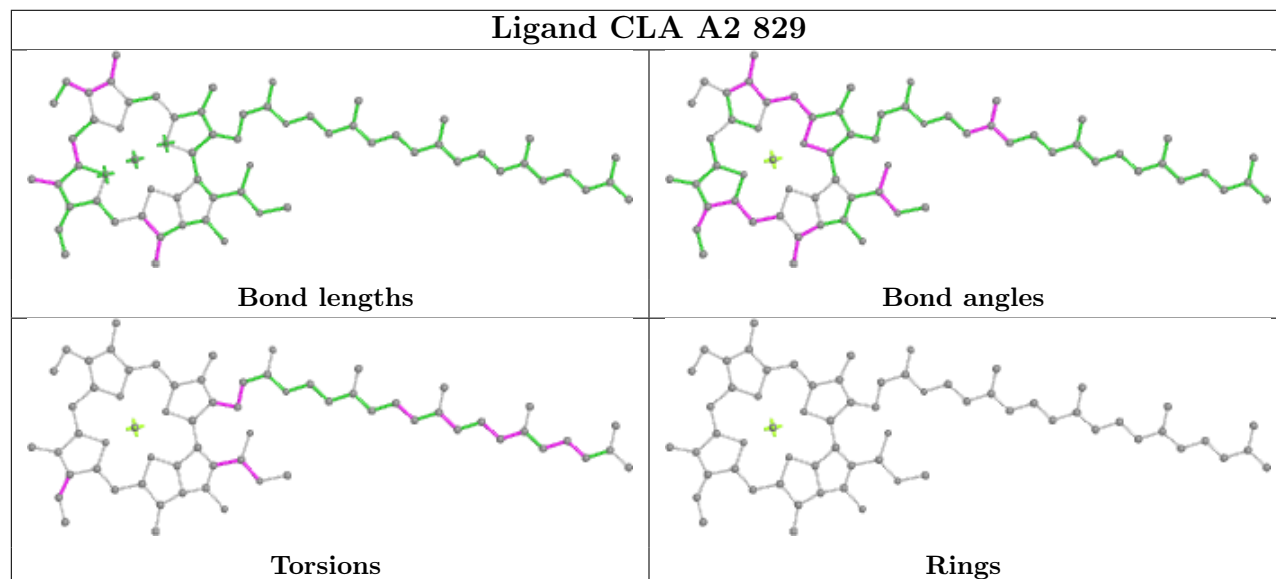
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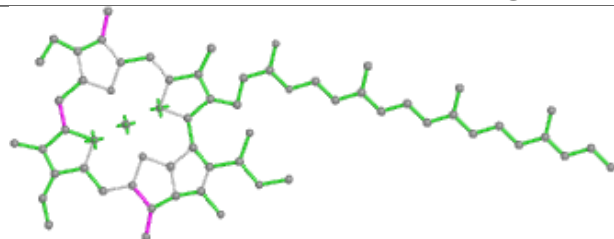
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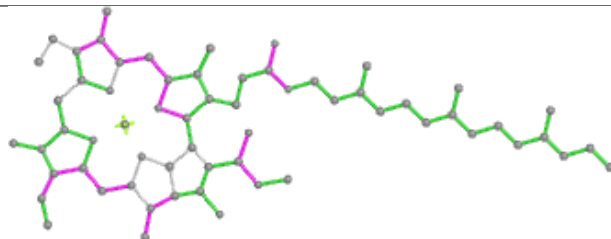
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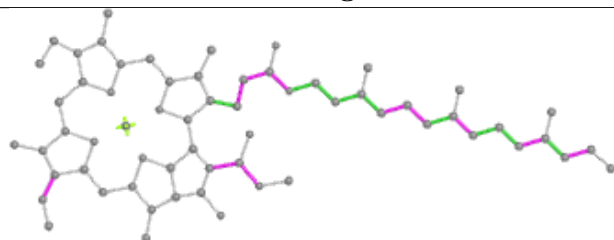
Ligand CLA A2 830



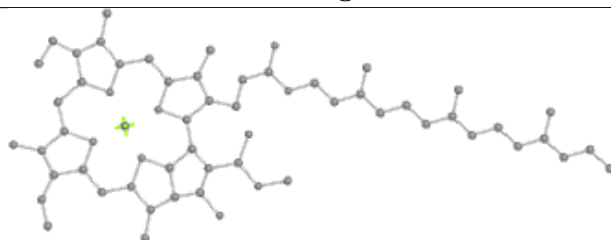
Bond lengths



Bond angles

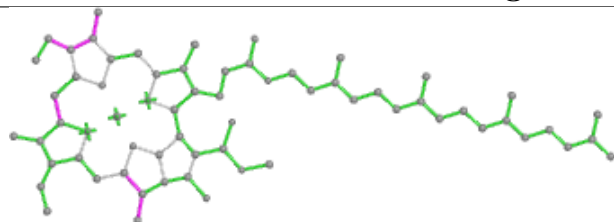


Torsions

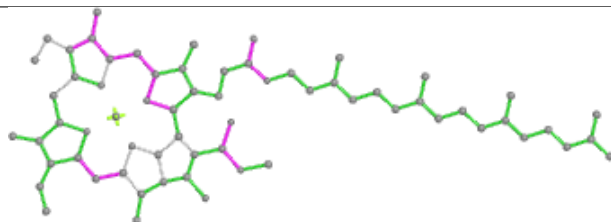


Rings

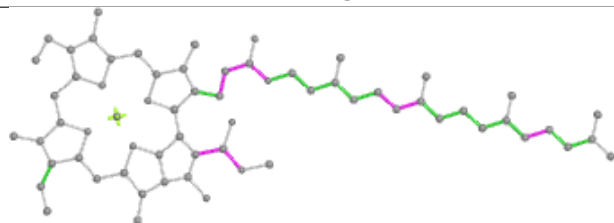
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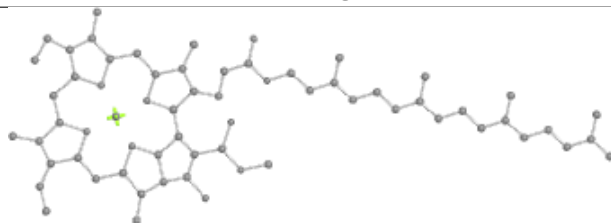
Bond lengths



Bond angles

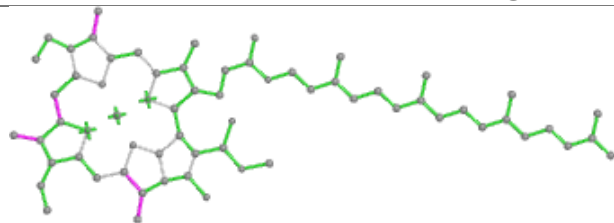


Torsions

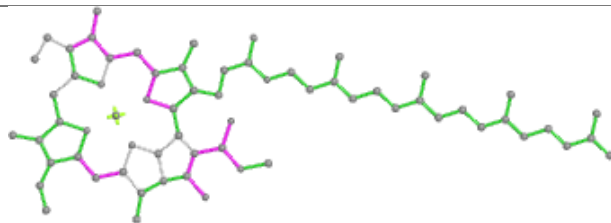


Rings

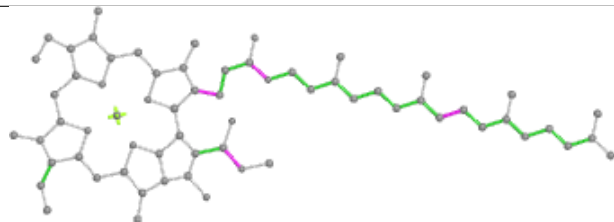
Ligand CLA A2 832



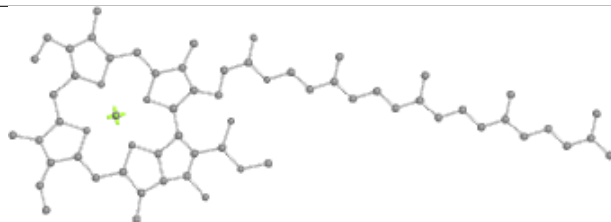
Bond lengths



Bond angles

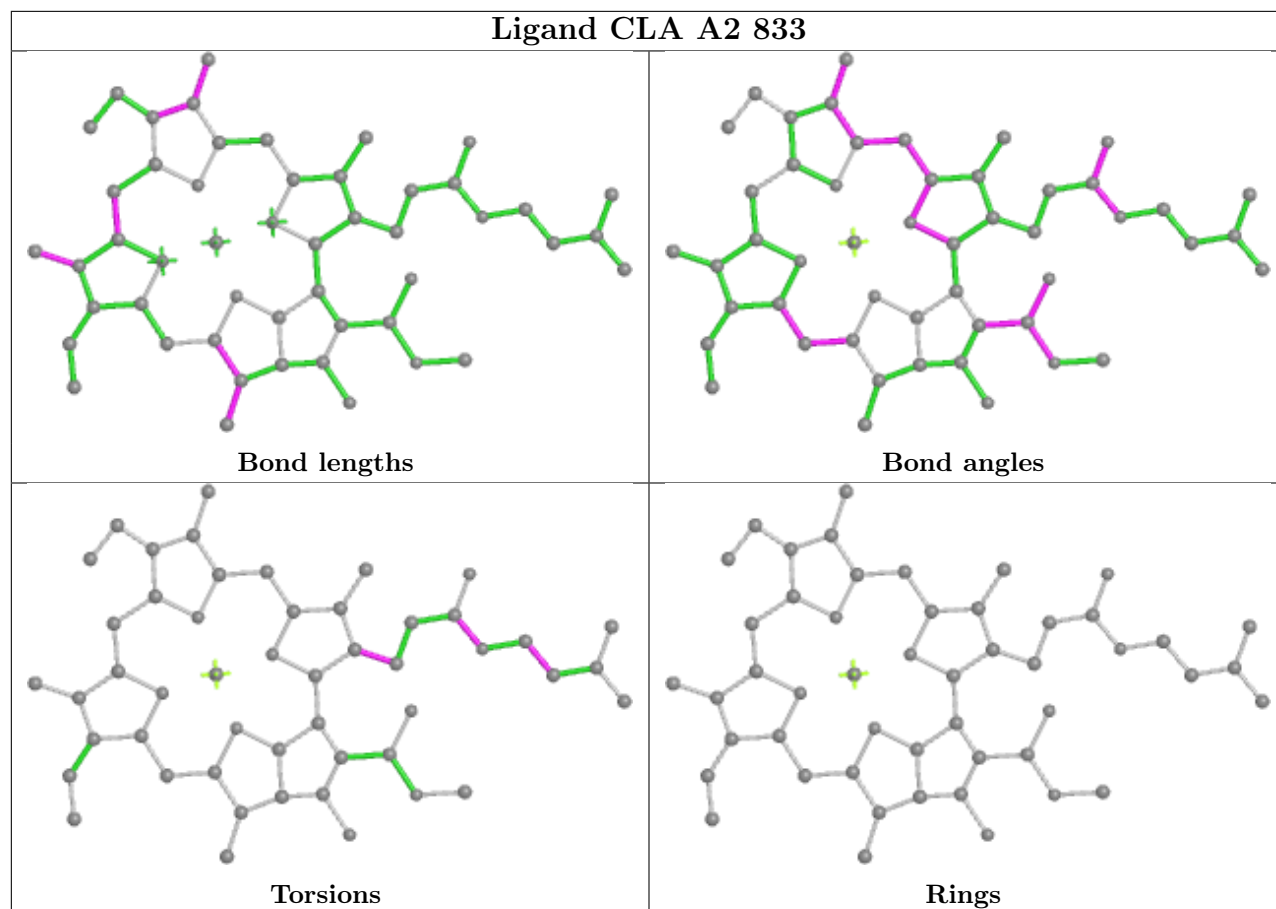


Torsions

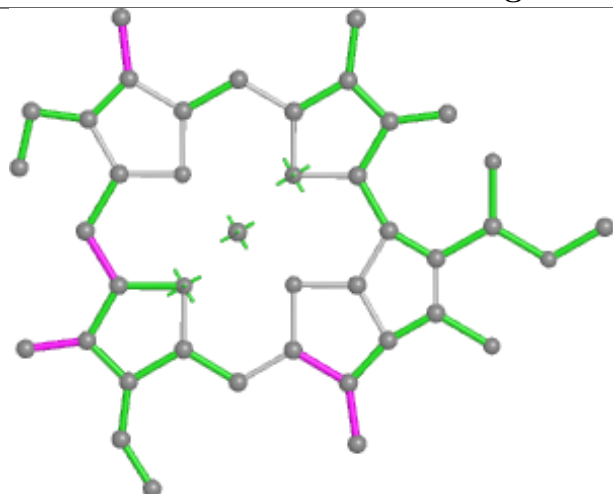


Rings

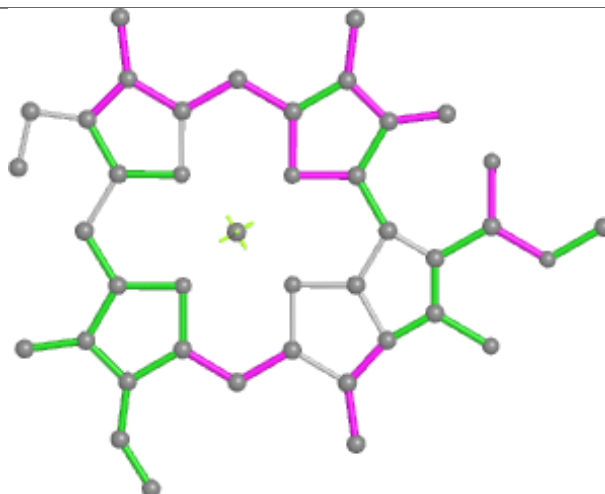
Ligand CLA A2 833



Ligand CLA A2 834



Bond lengths



Bond angles

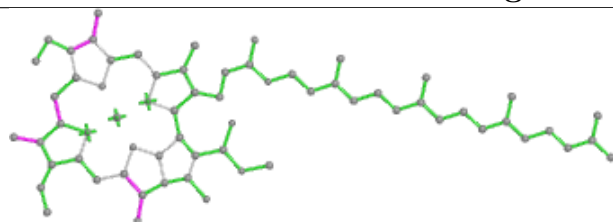


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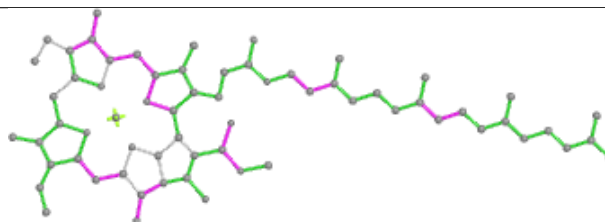


Rings

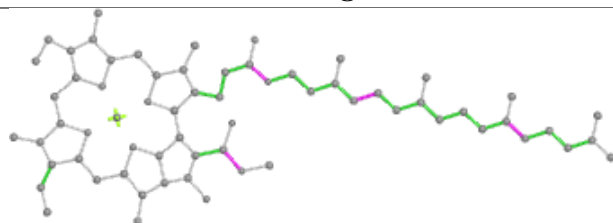
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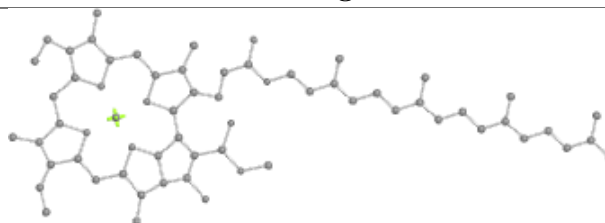
Bond lengths



Bond angles

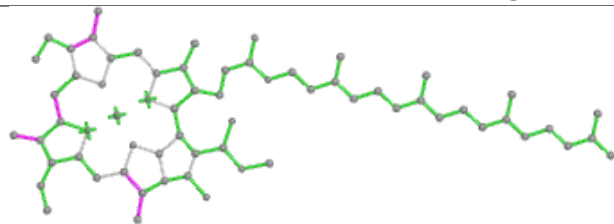


Torsions

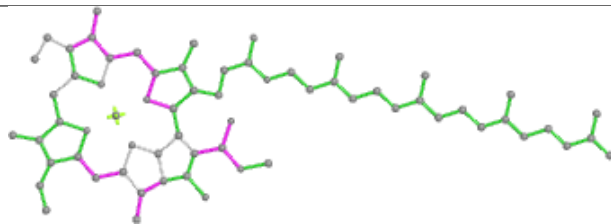


Rings

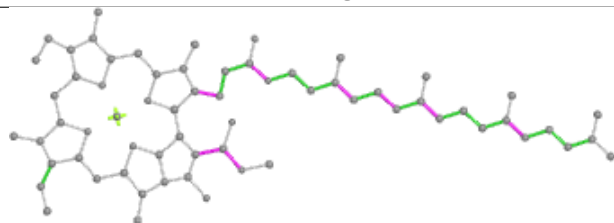
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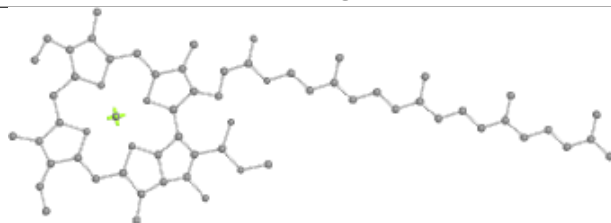
Bond lengths



Bond angles

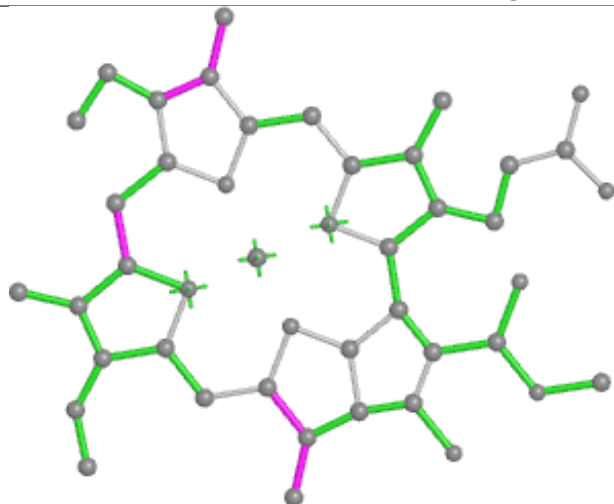


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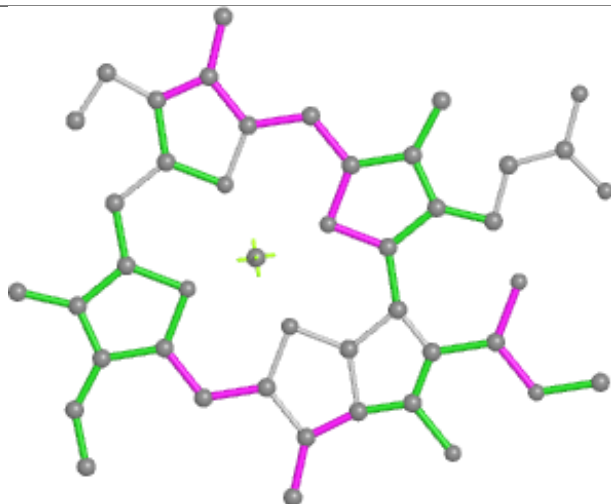


Rings

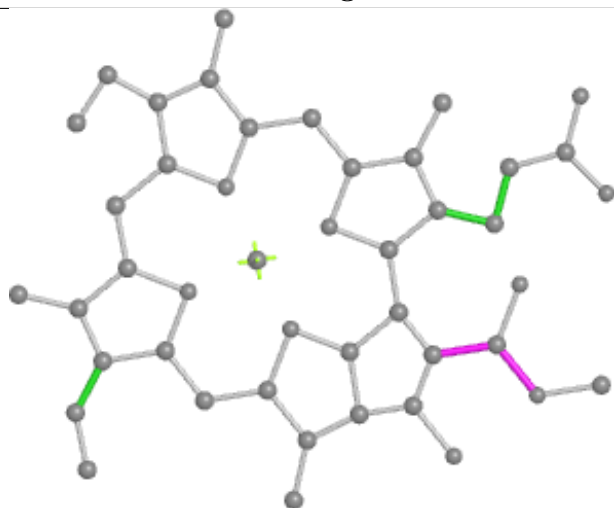
Ligand CLA A2 837



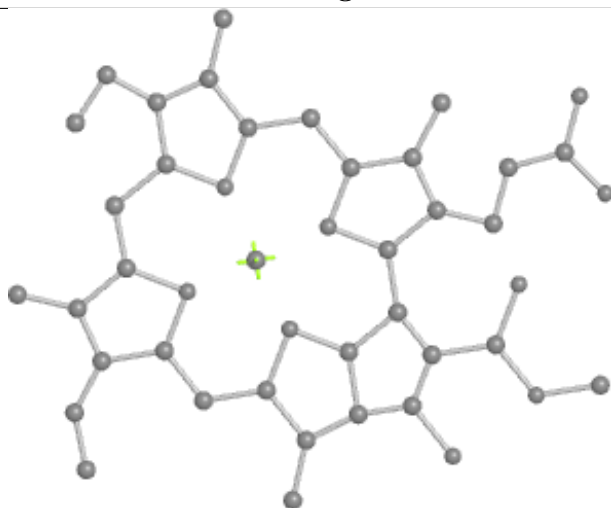
Bond lengths



Bond angles

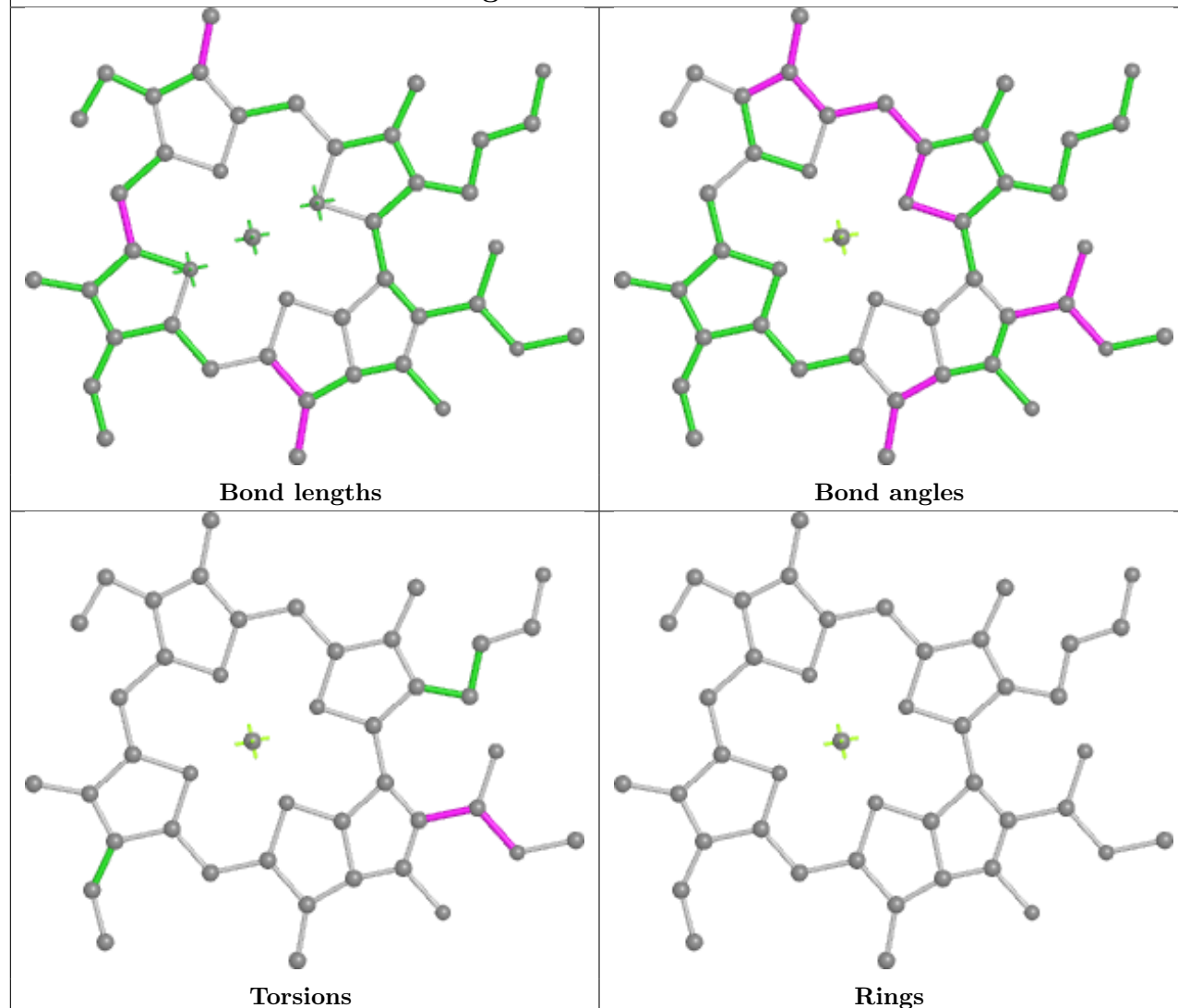


Torsions

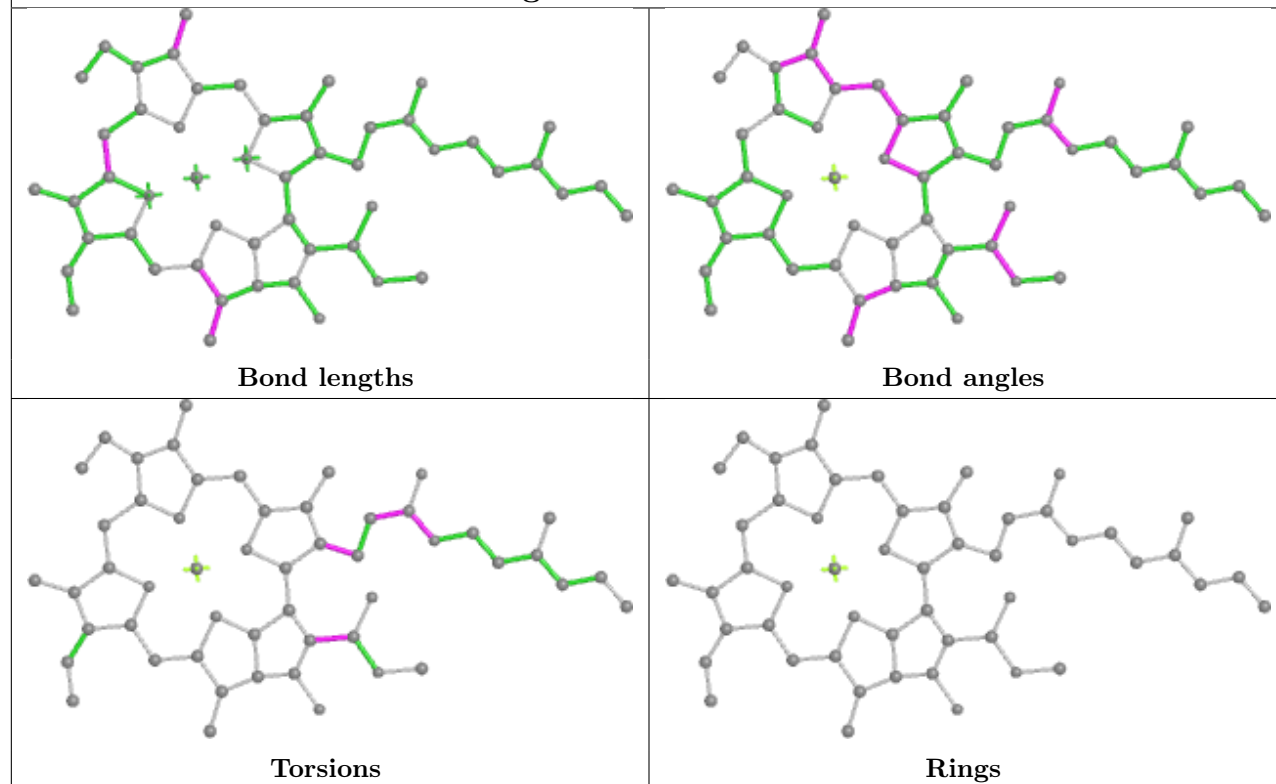


Rings

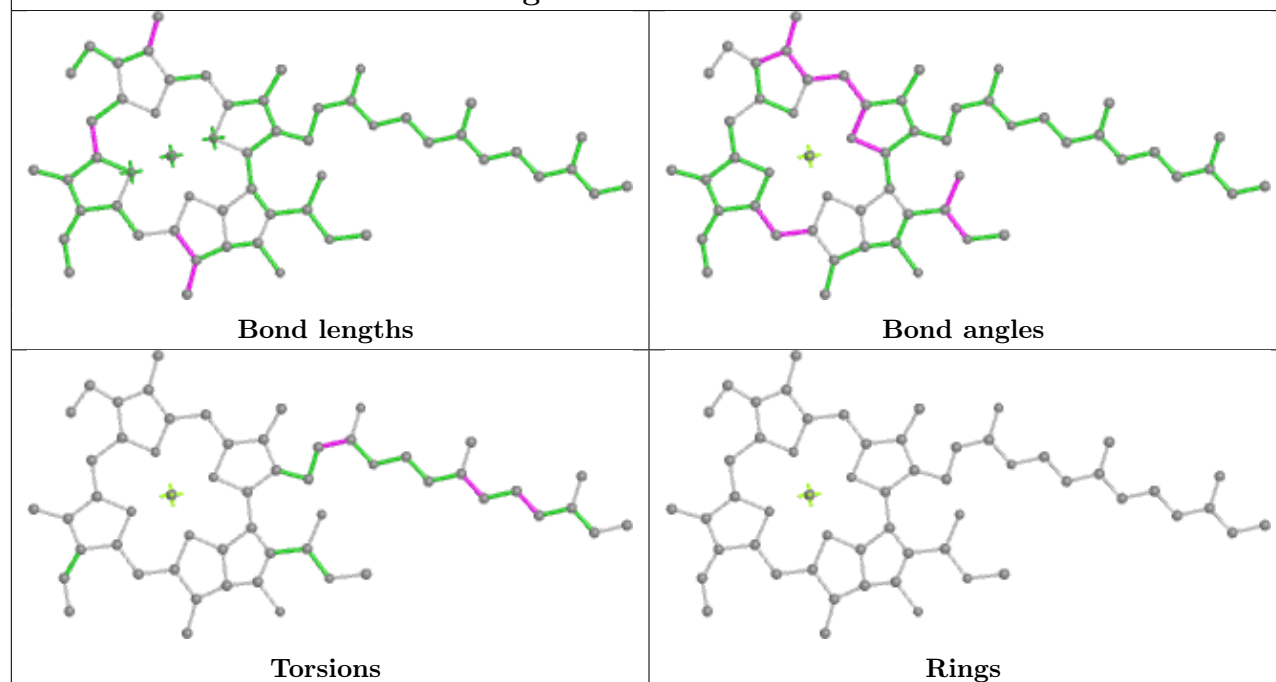
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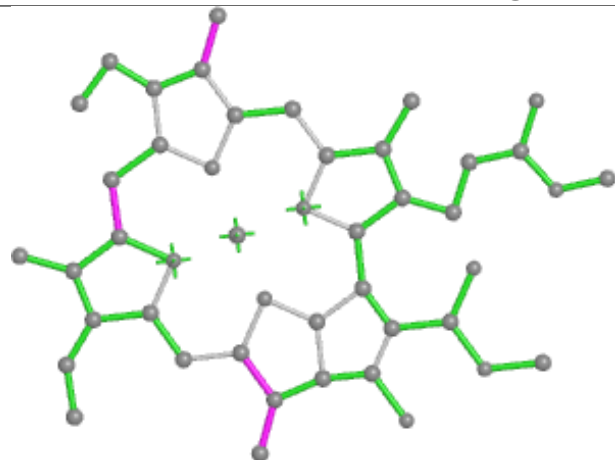
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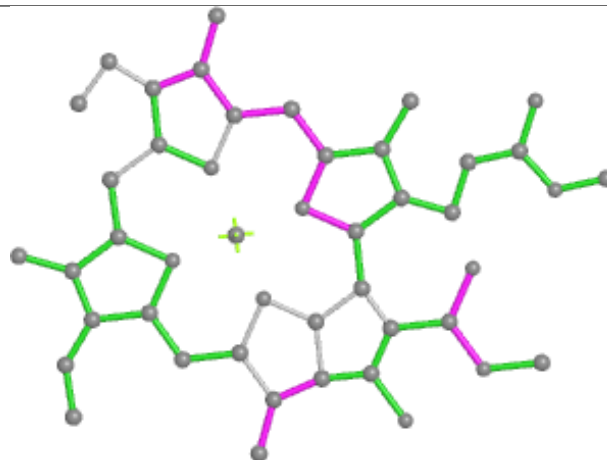
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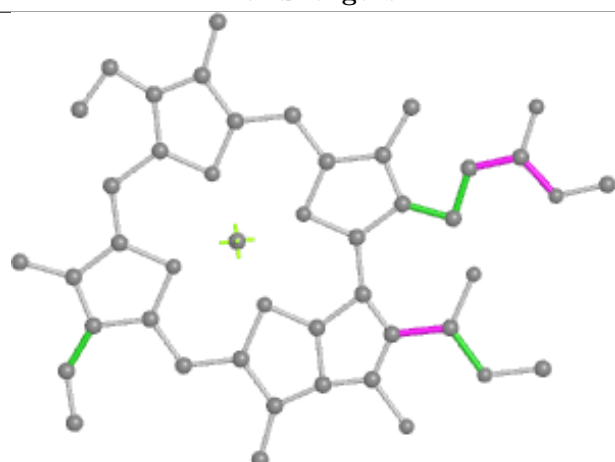
Ligand CLA A2 841



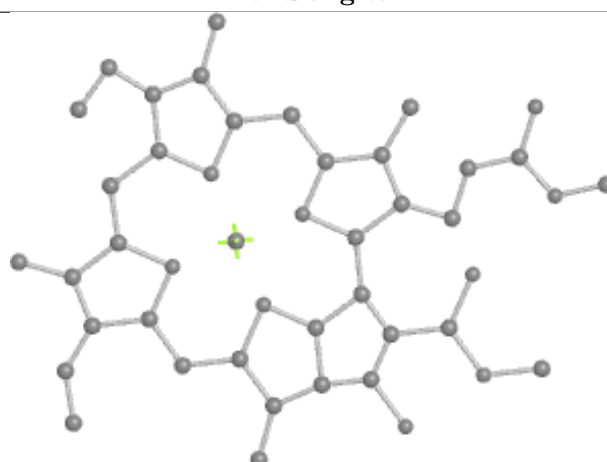
Bond lengths



Bond angles

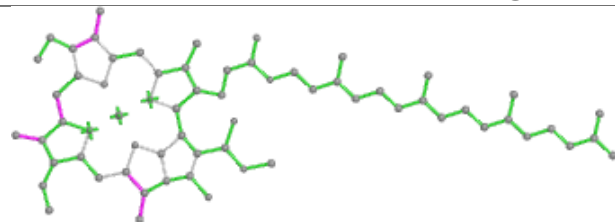


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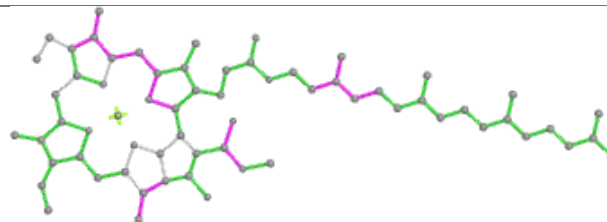


Rings

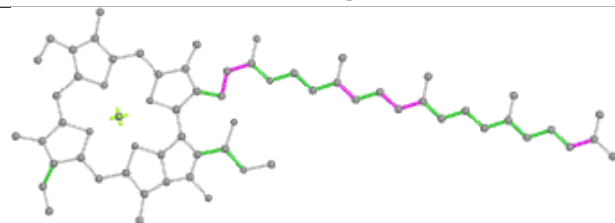
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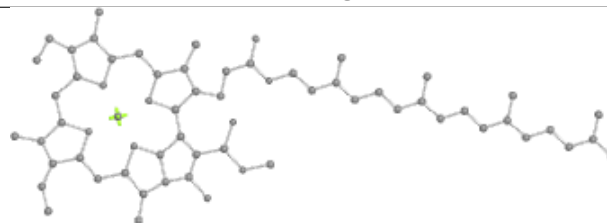
Bond lengths



Bond angles

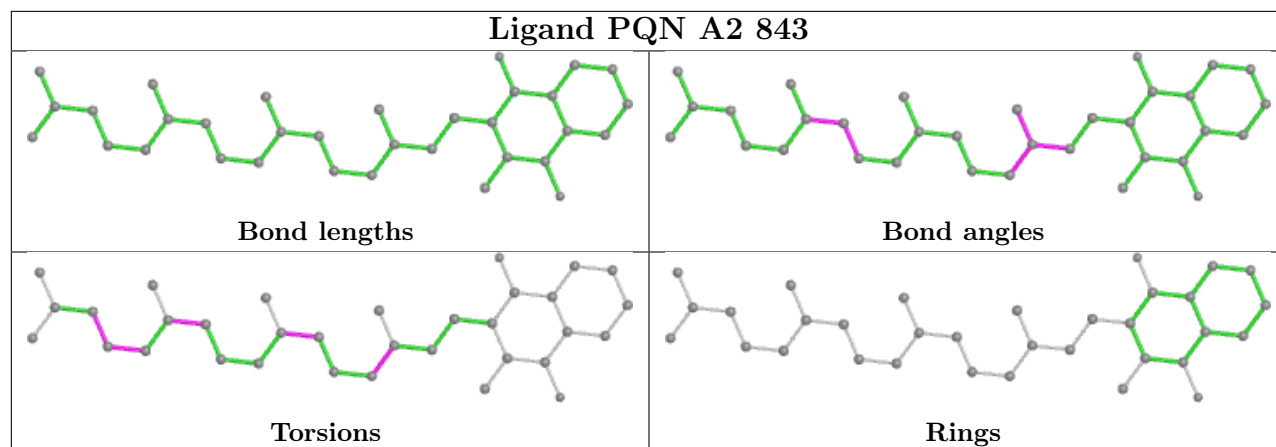


Torsions

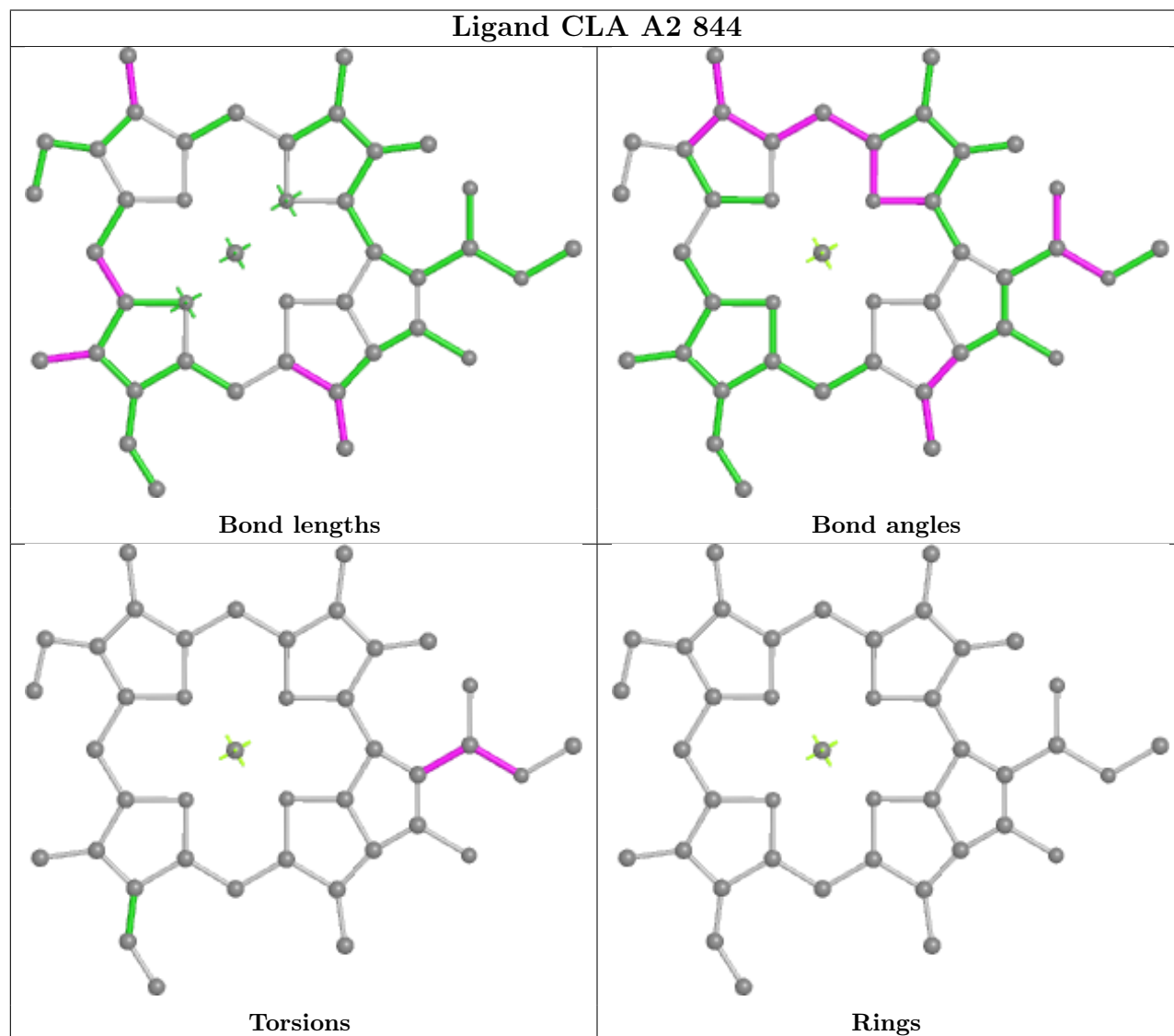


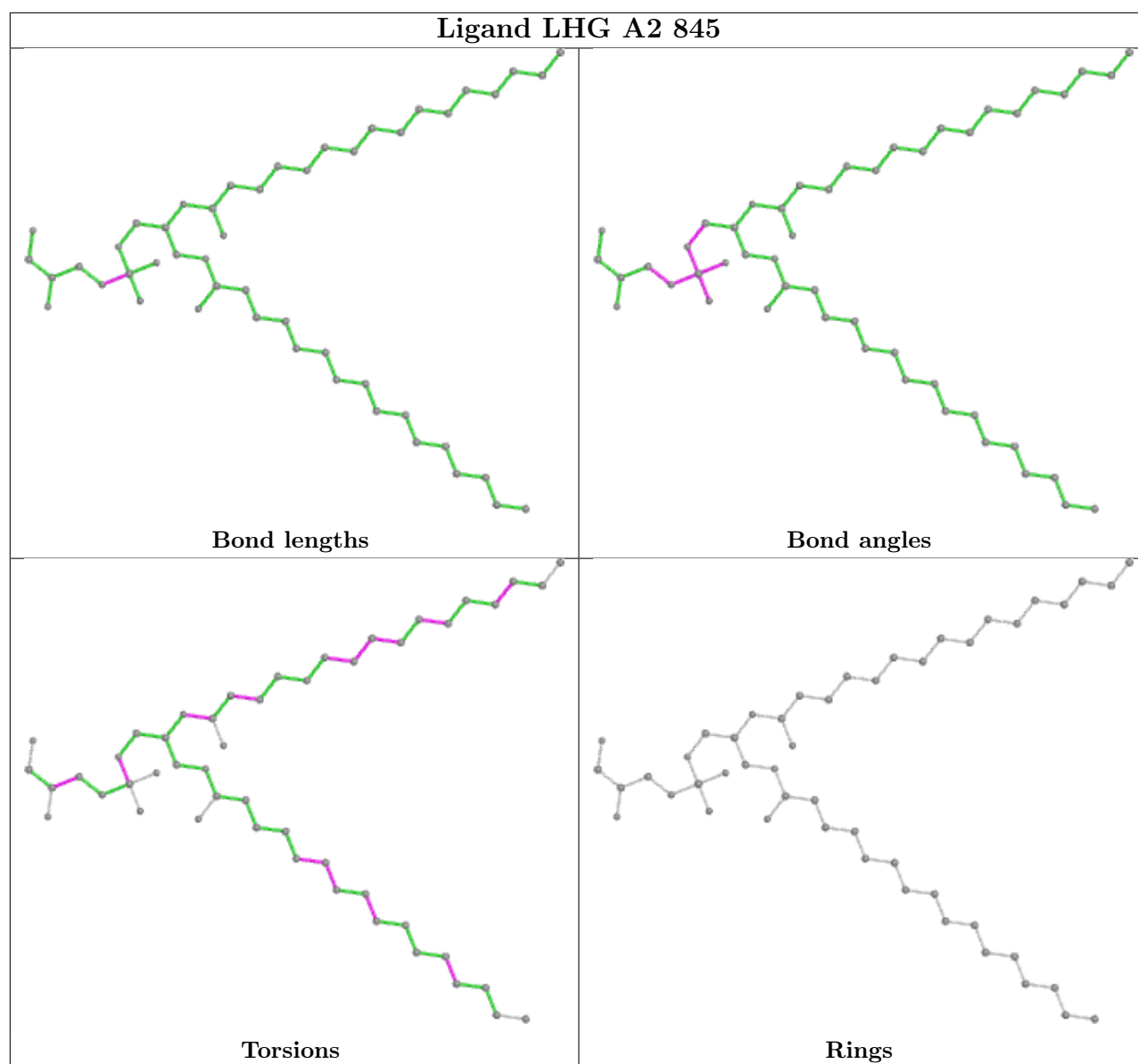
Rings

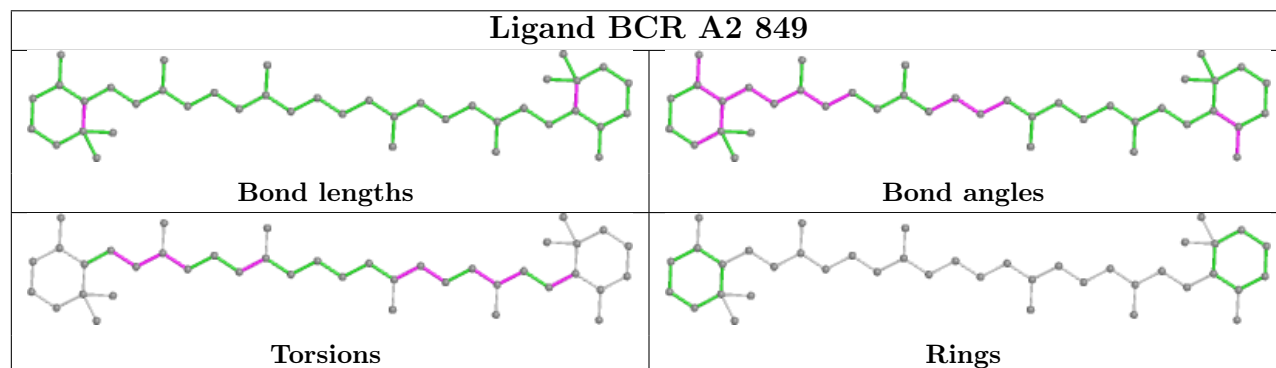
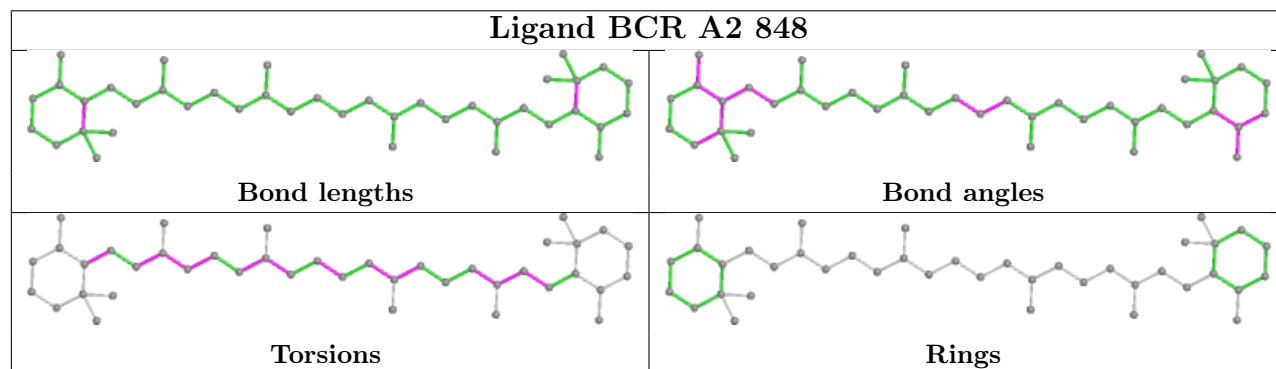
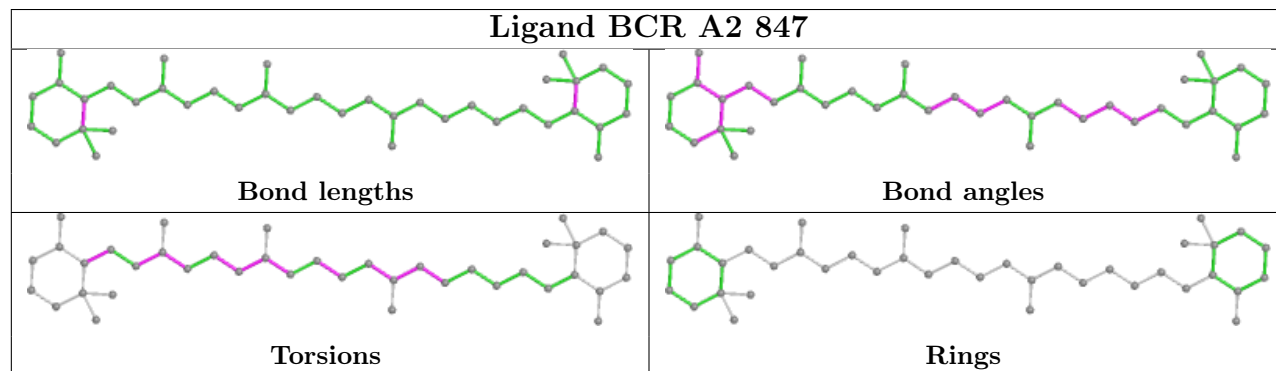
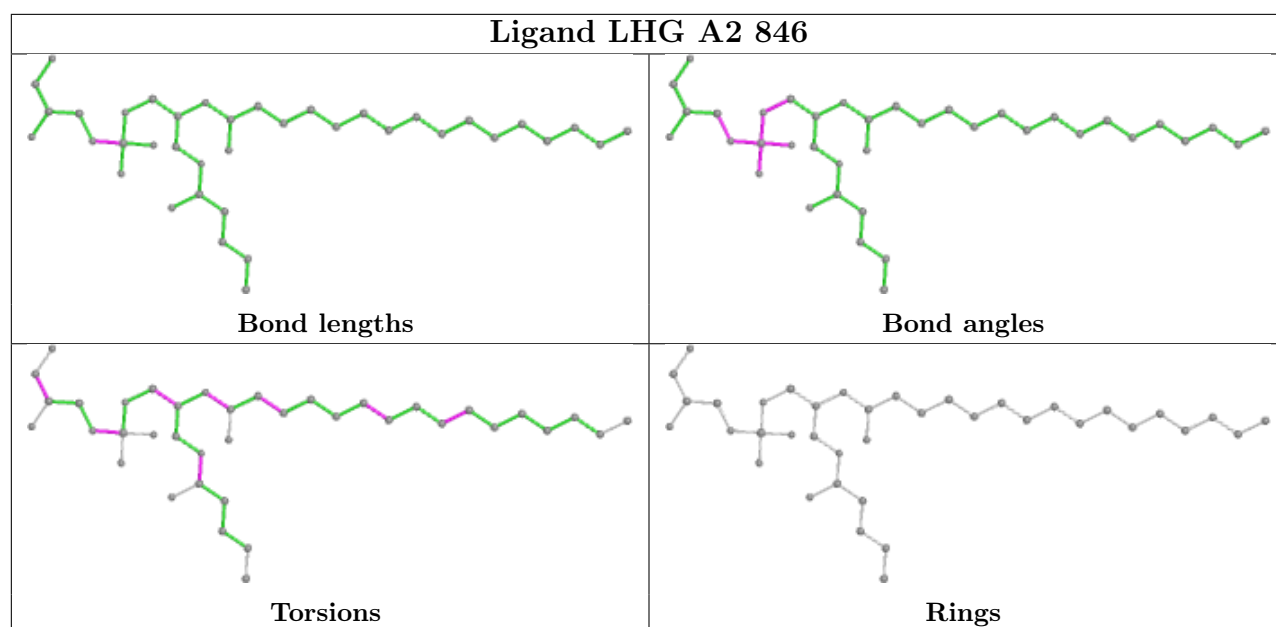
Ligand PQN A2 843

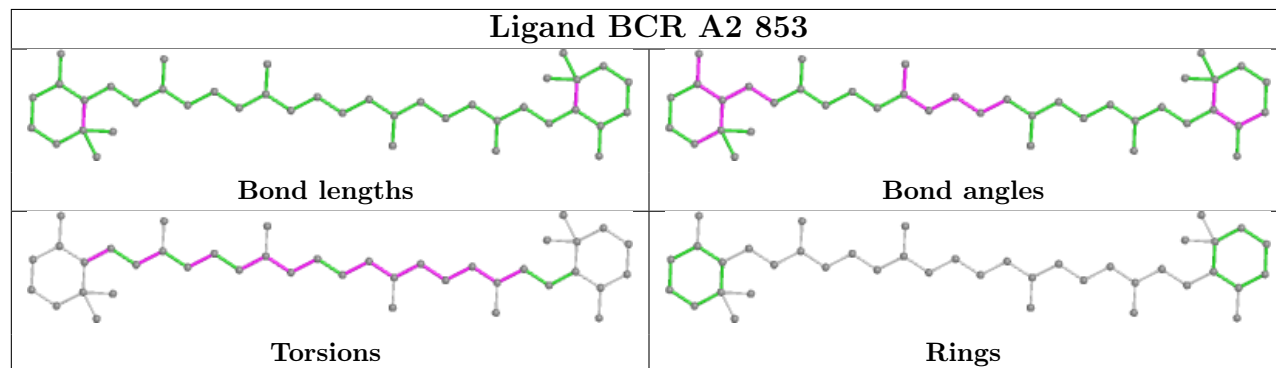
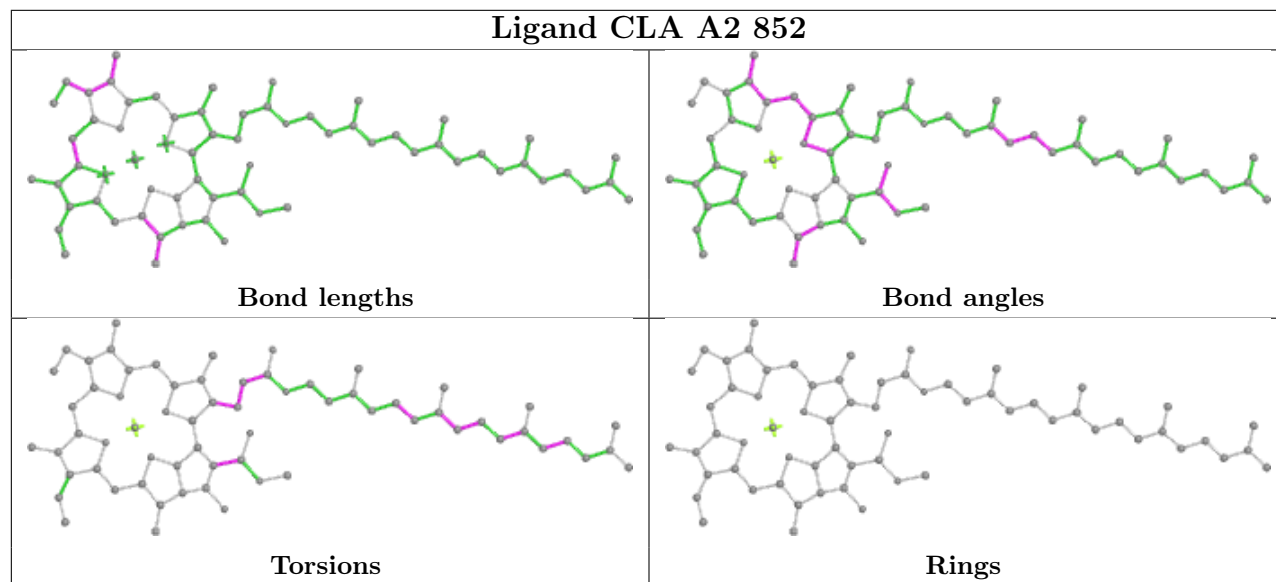
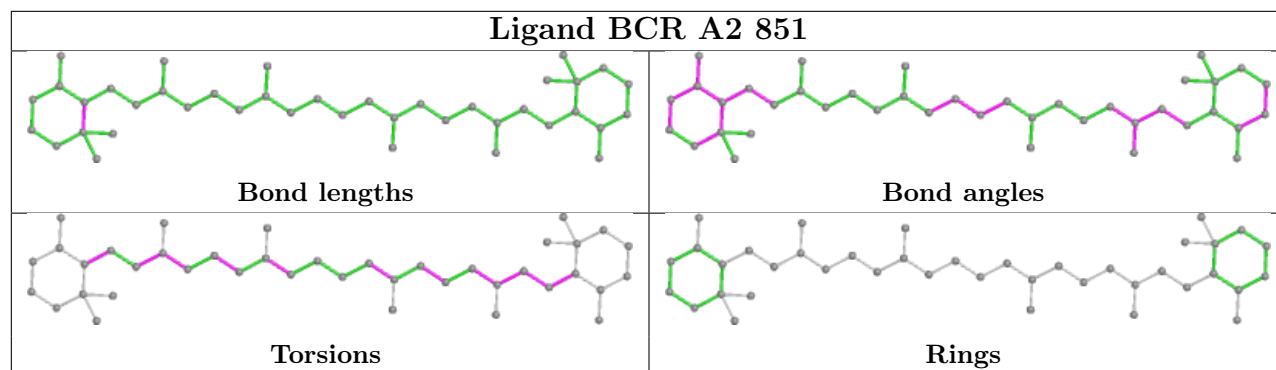
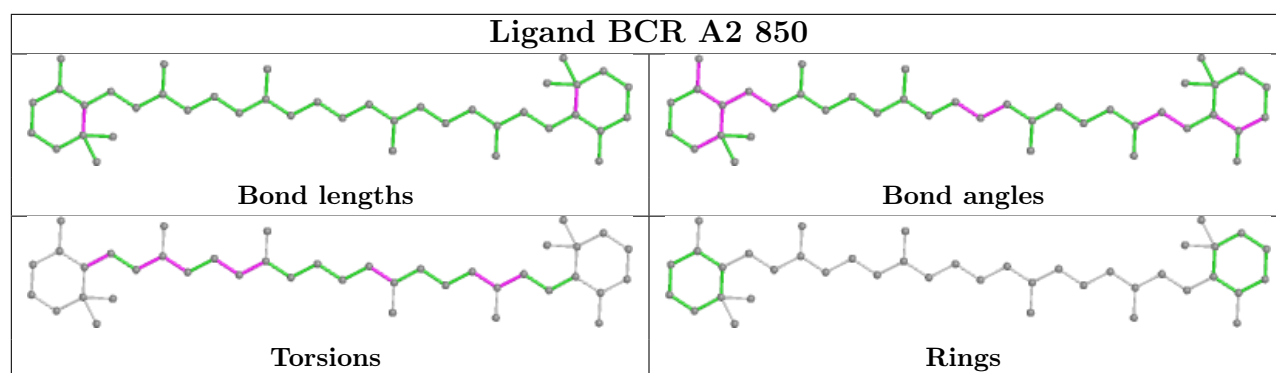


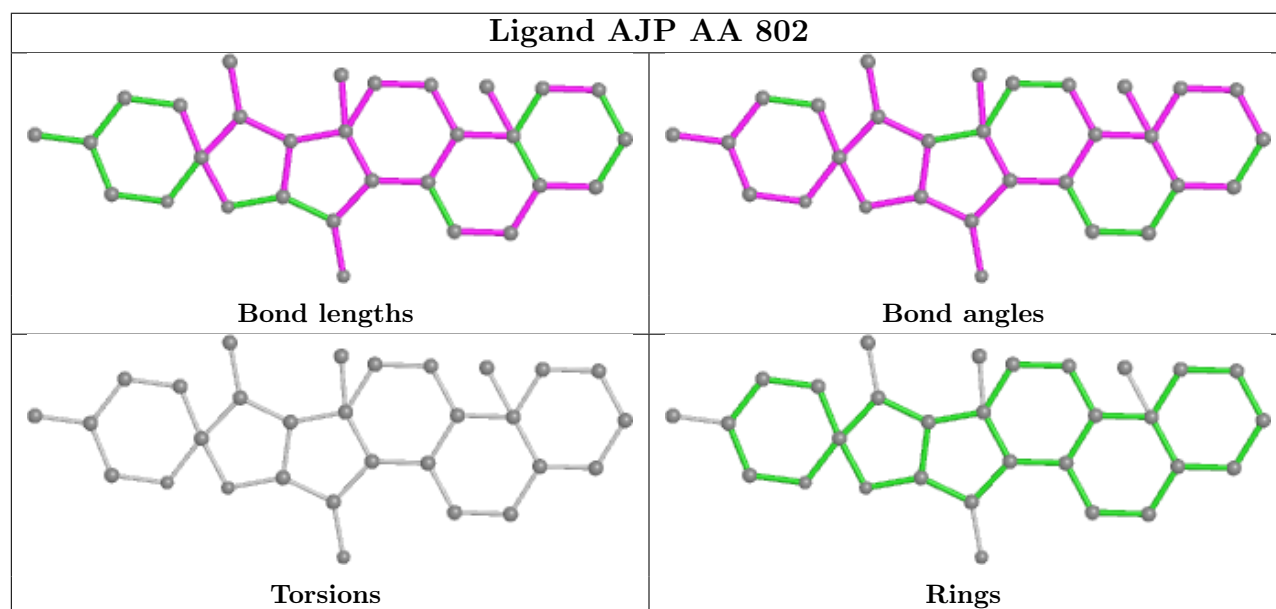
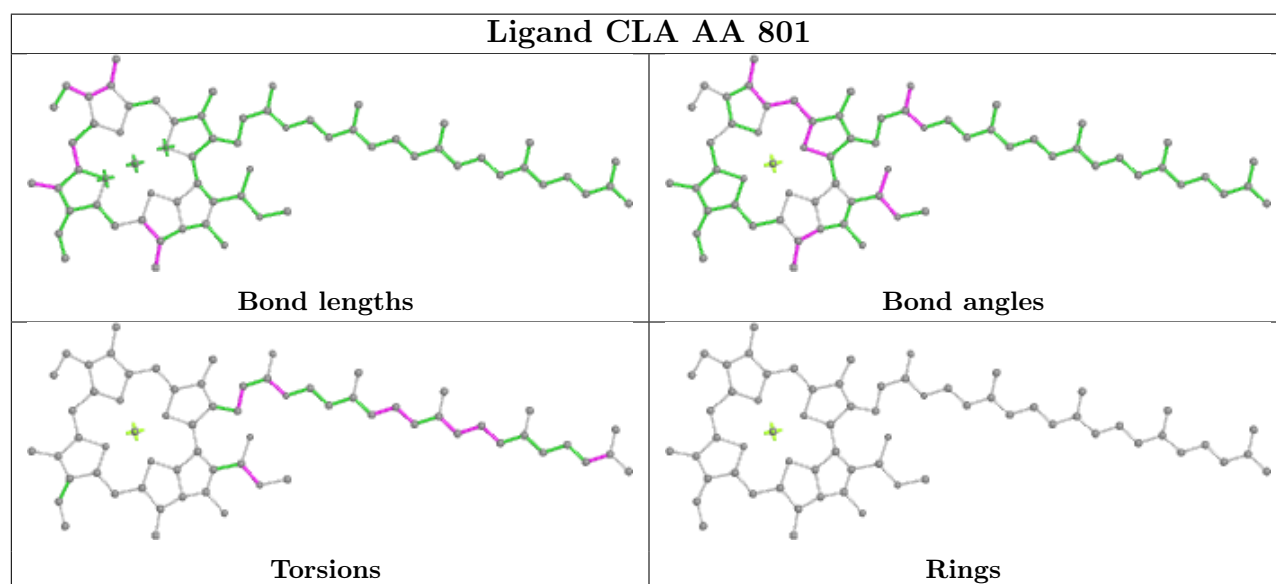
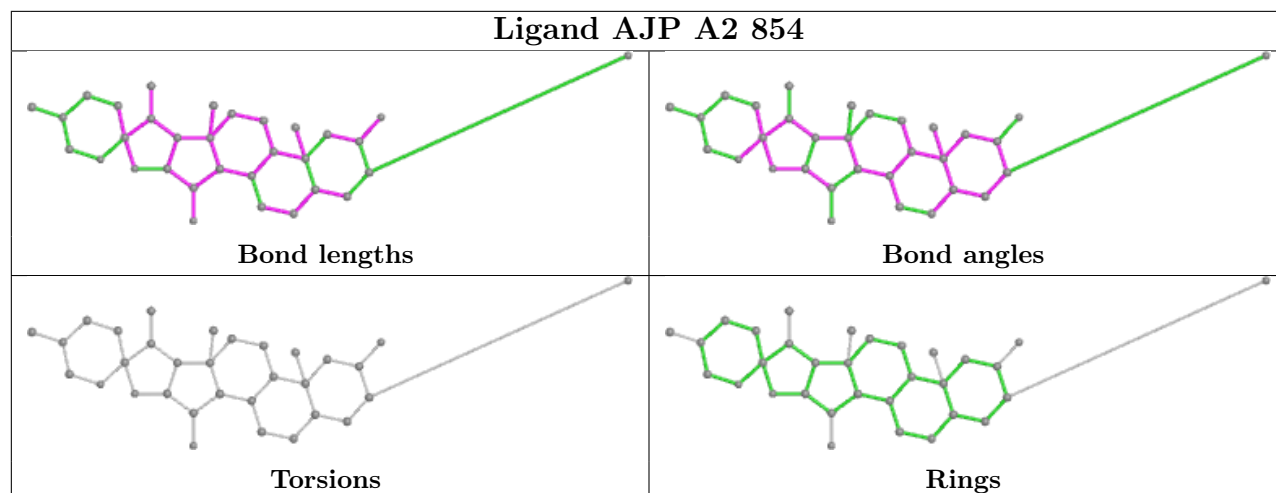
Ligand CLA A2 844

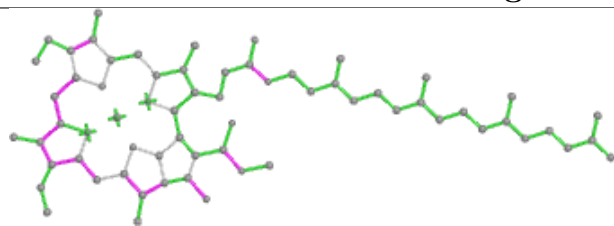
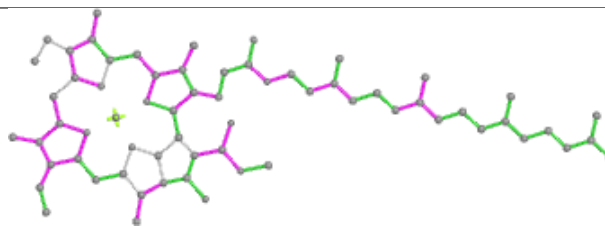
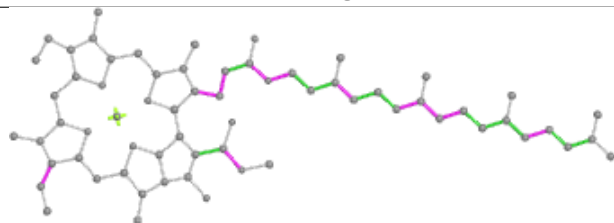
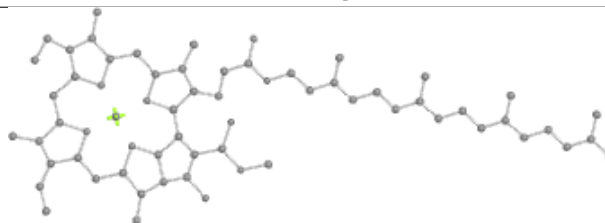
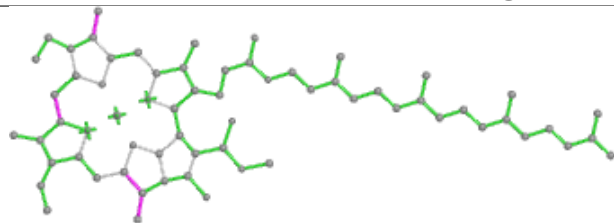
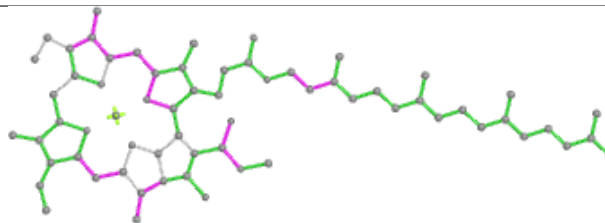
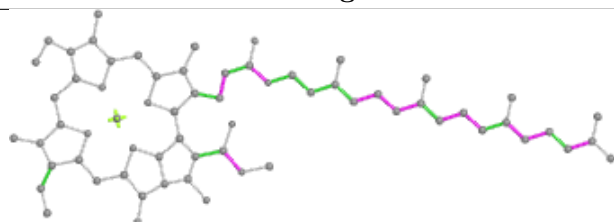
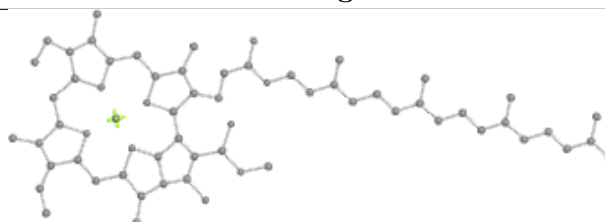




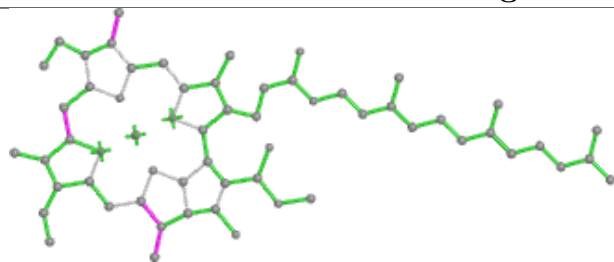




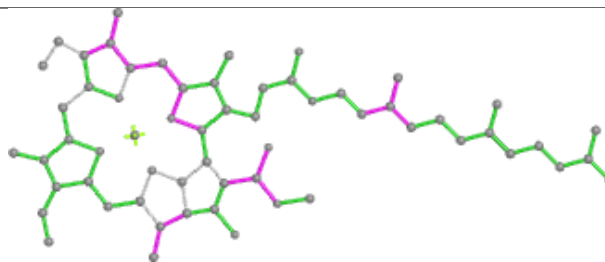


Ligand CL0 AA 803**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA AA 804****Bond lengths****Bond angles****Torsions****Rings**

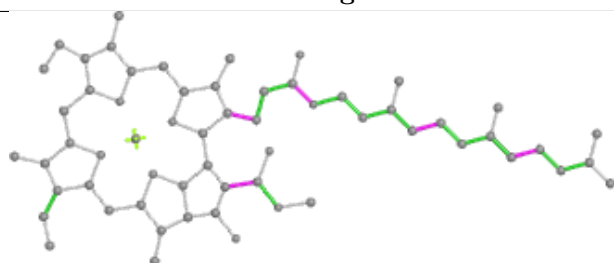
Ligand CLA AA 805



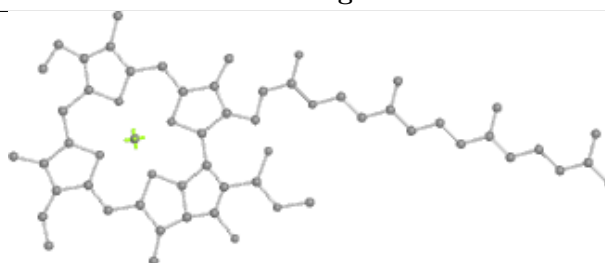
Bond lengths



Bond angles

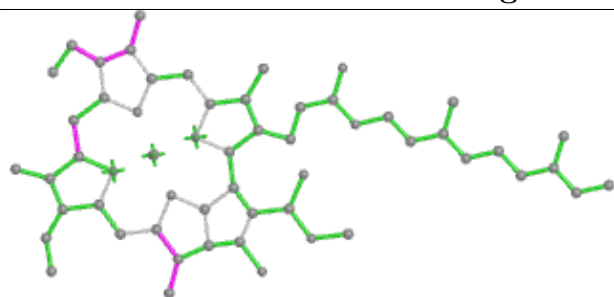


Torsions

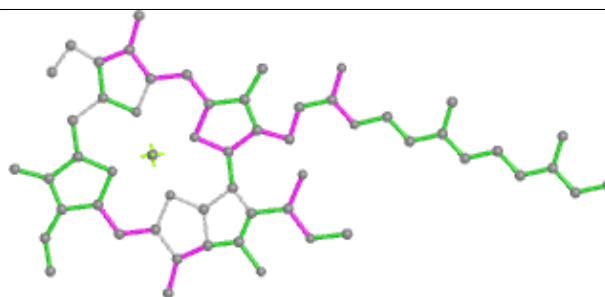


Rings

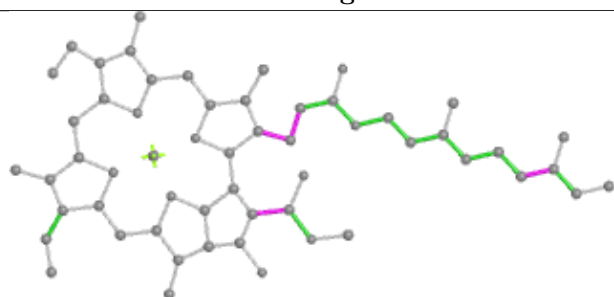
Ligand CLA AA 806



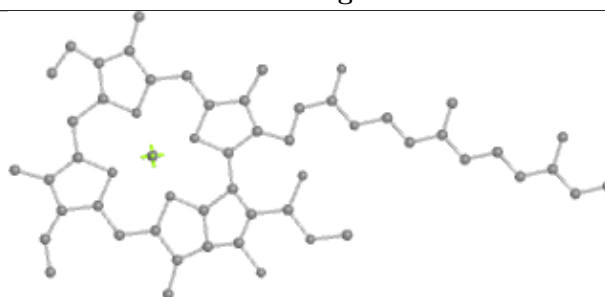
Bond lengths



Bond angles

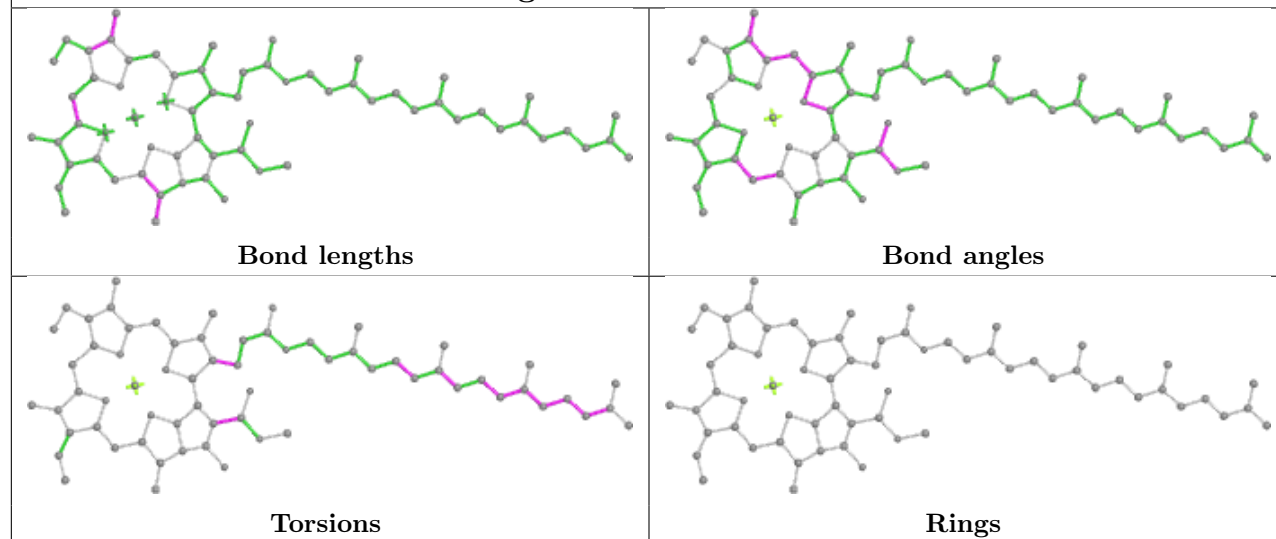


Torsions

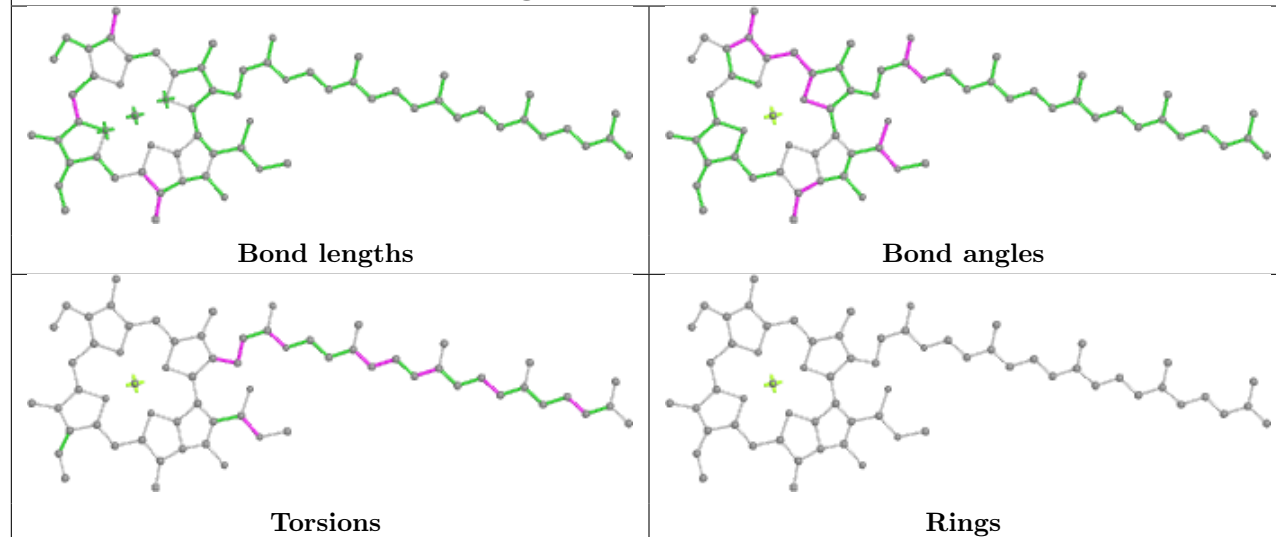


Rings

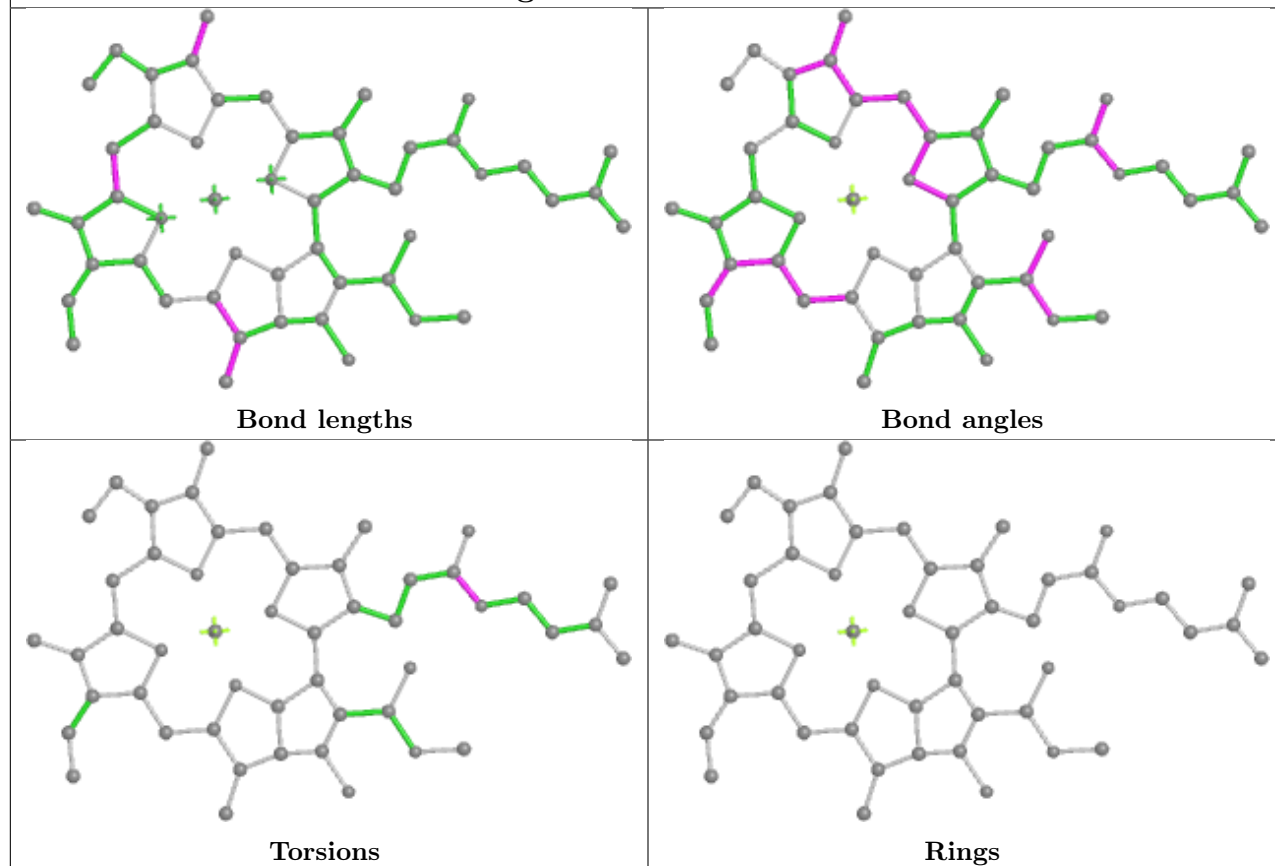
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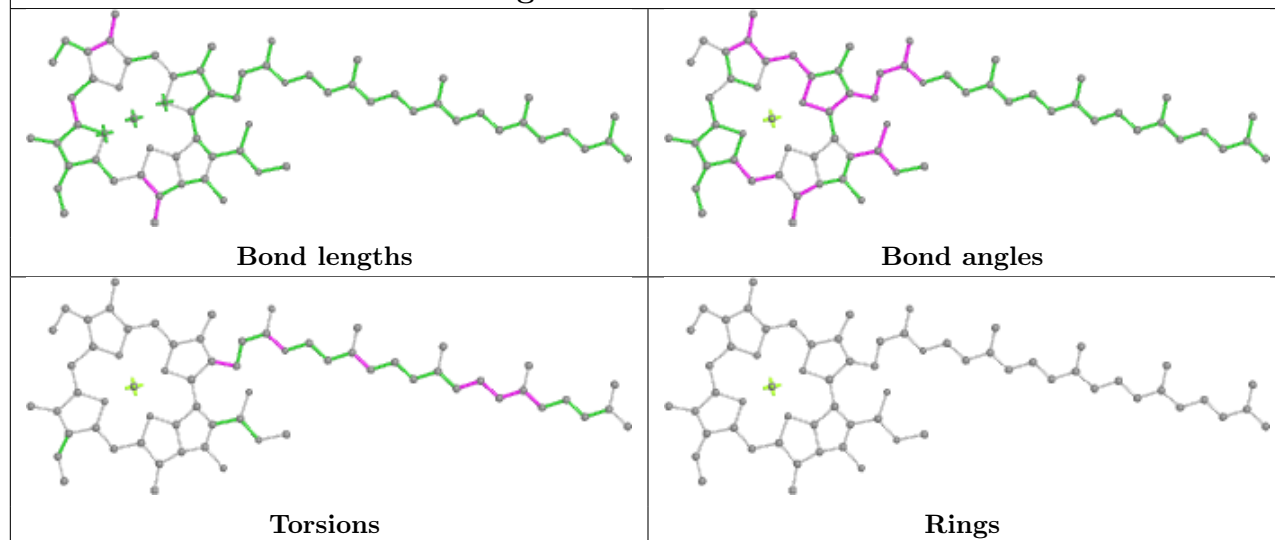
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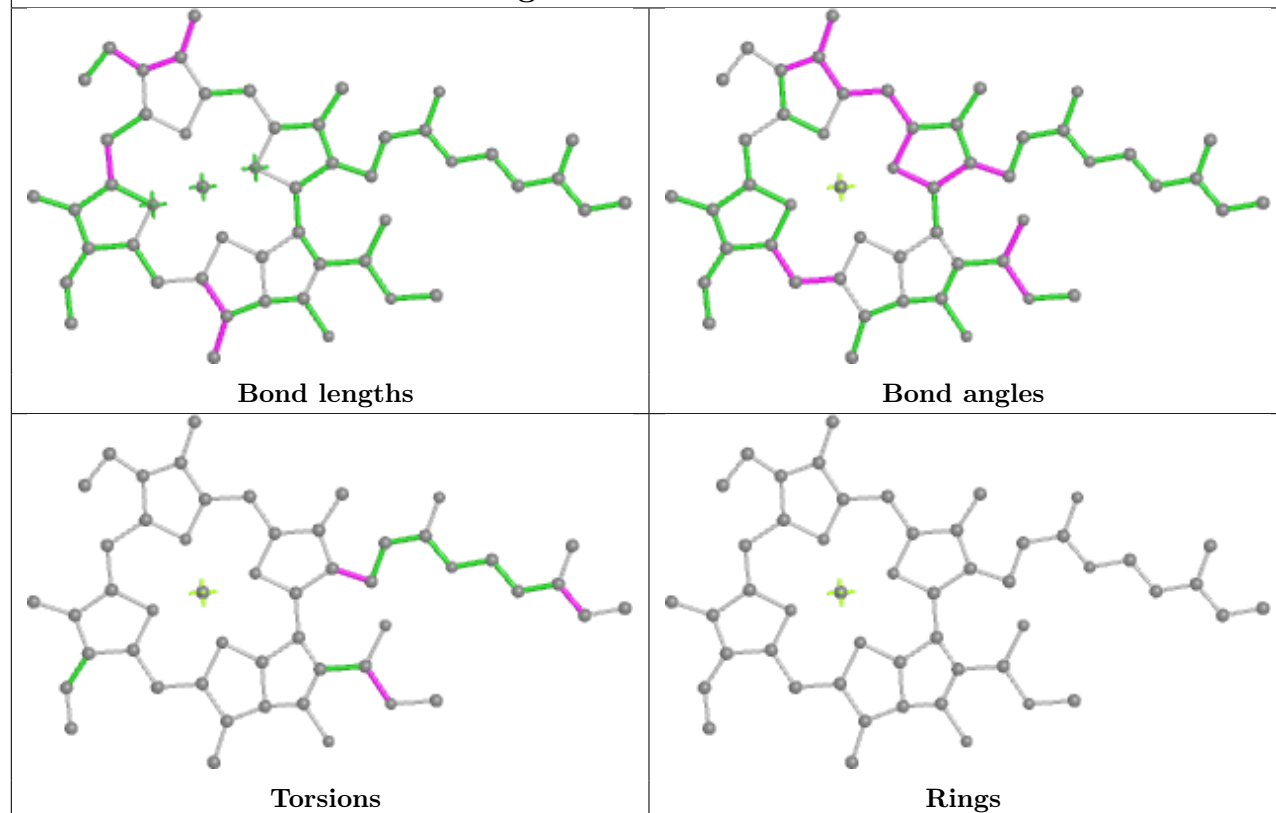
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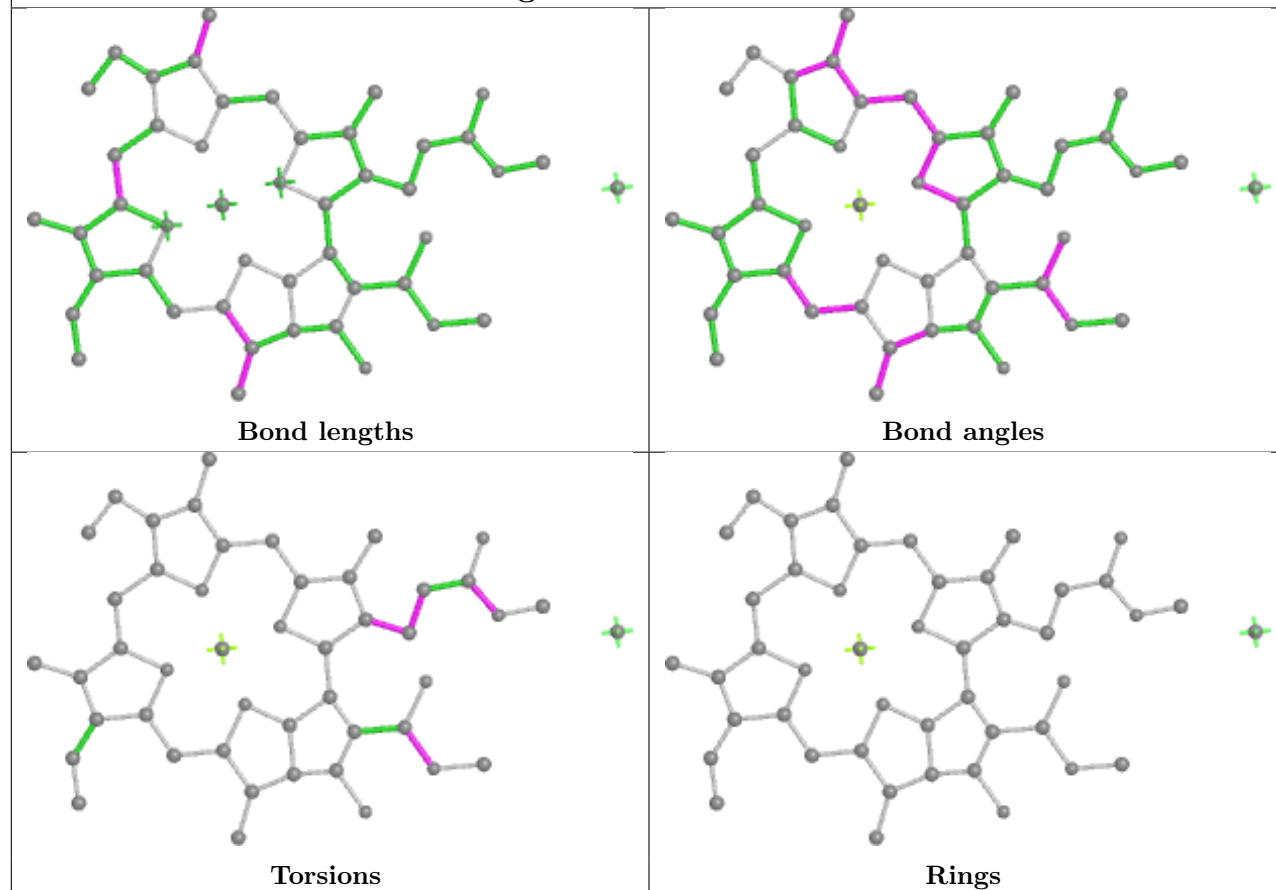
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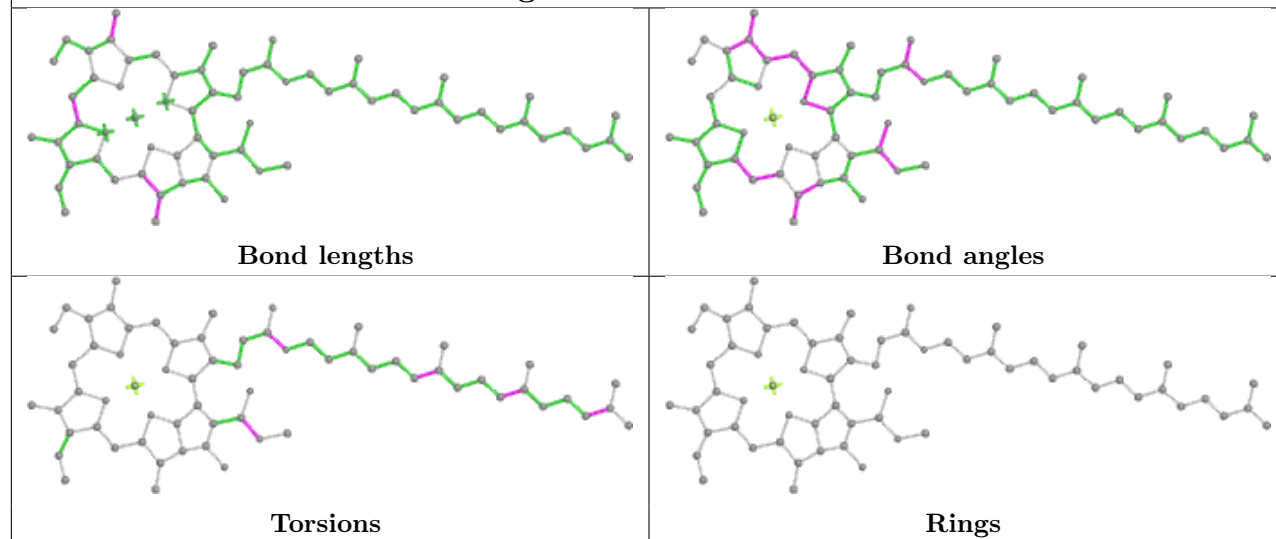
Ligand CLA AA 811



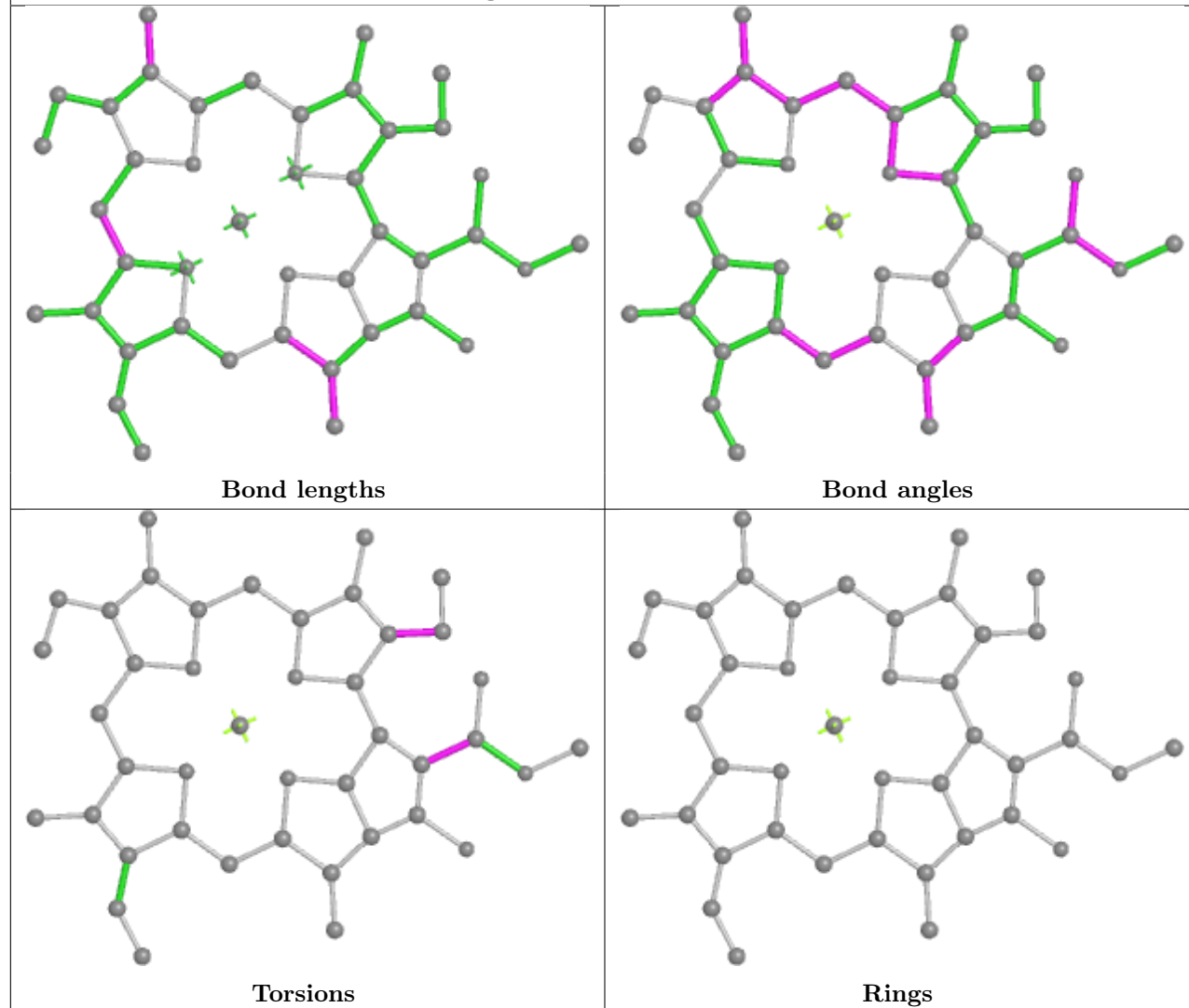
Ligand CLA AA 812



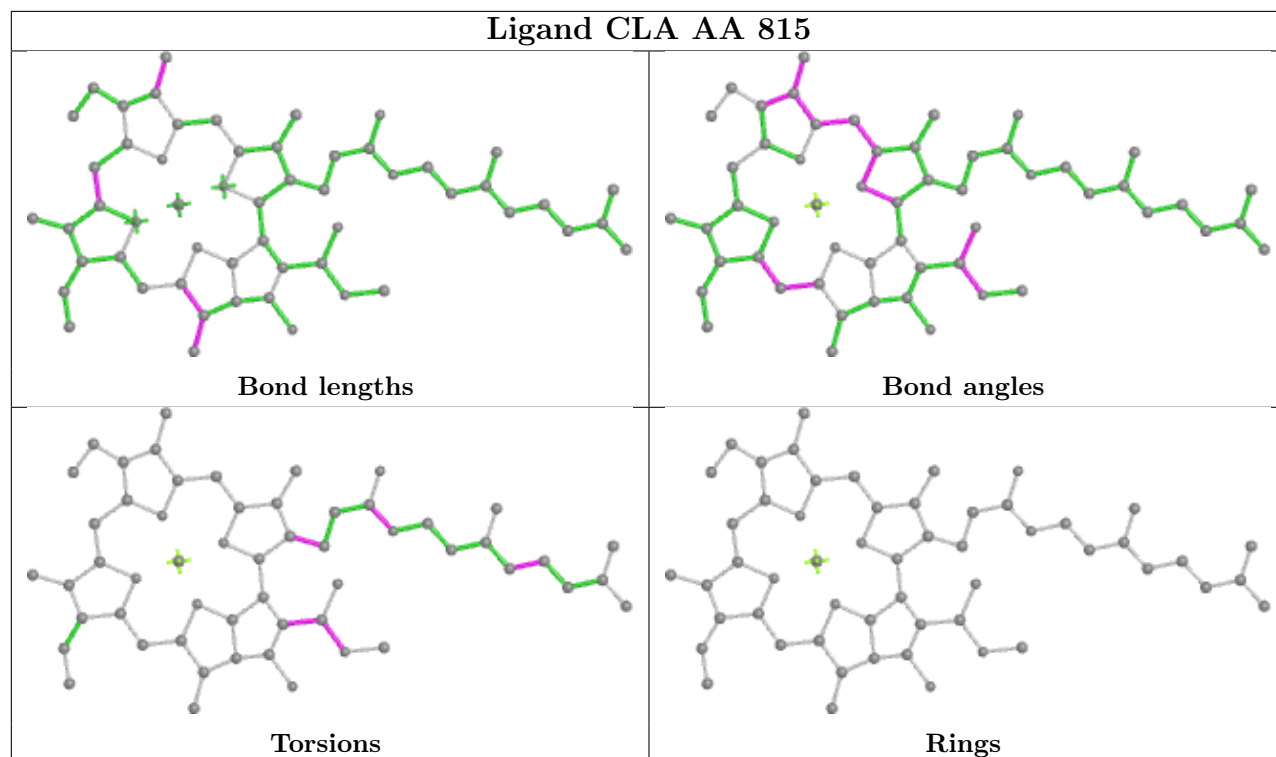
Ligand CLA AA 813



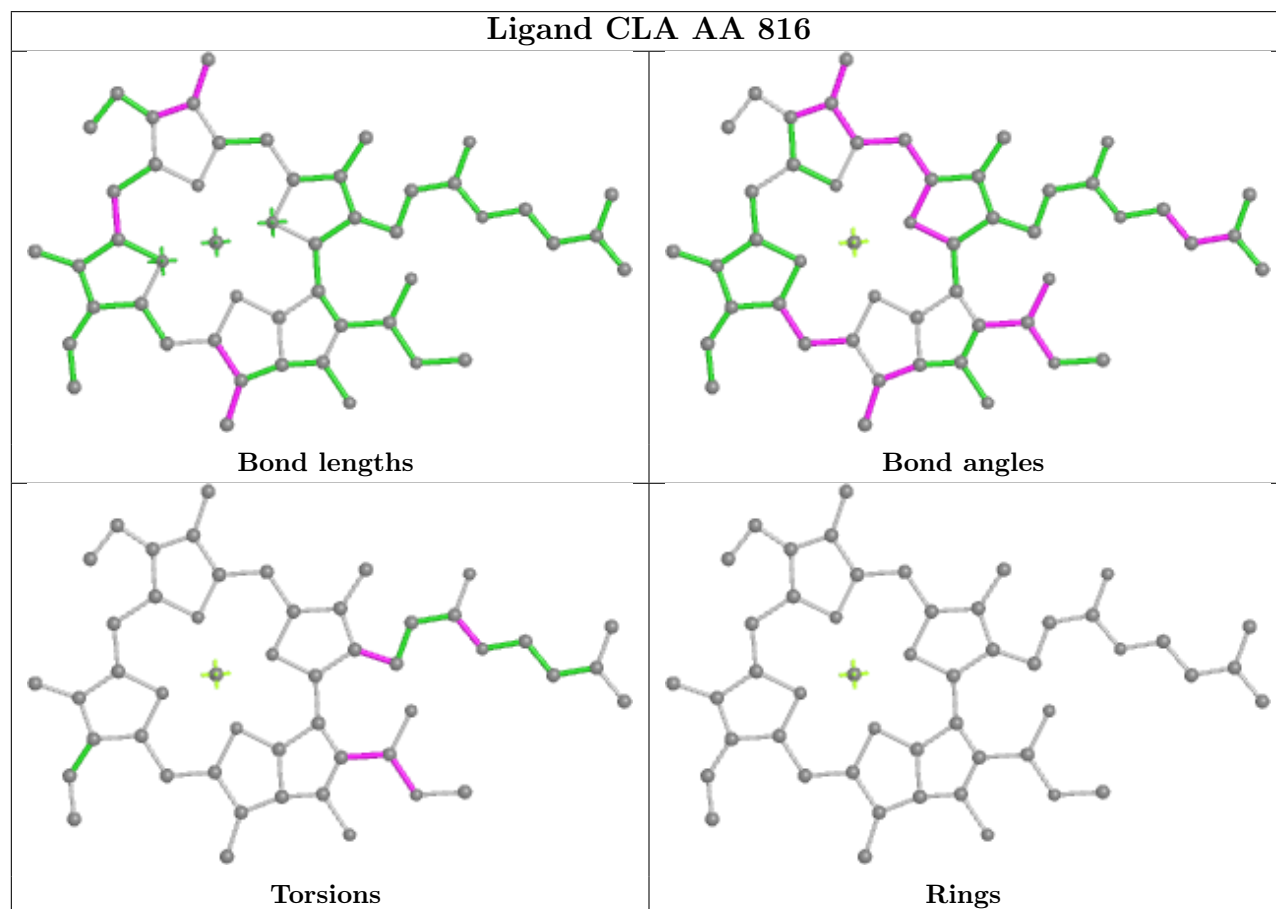
Ligand CLA AA 814



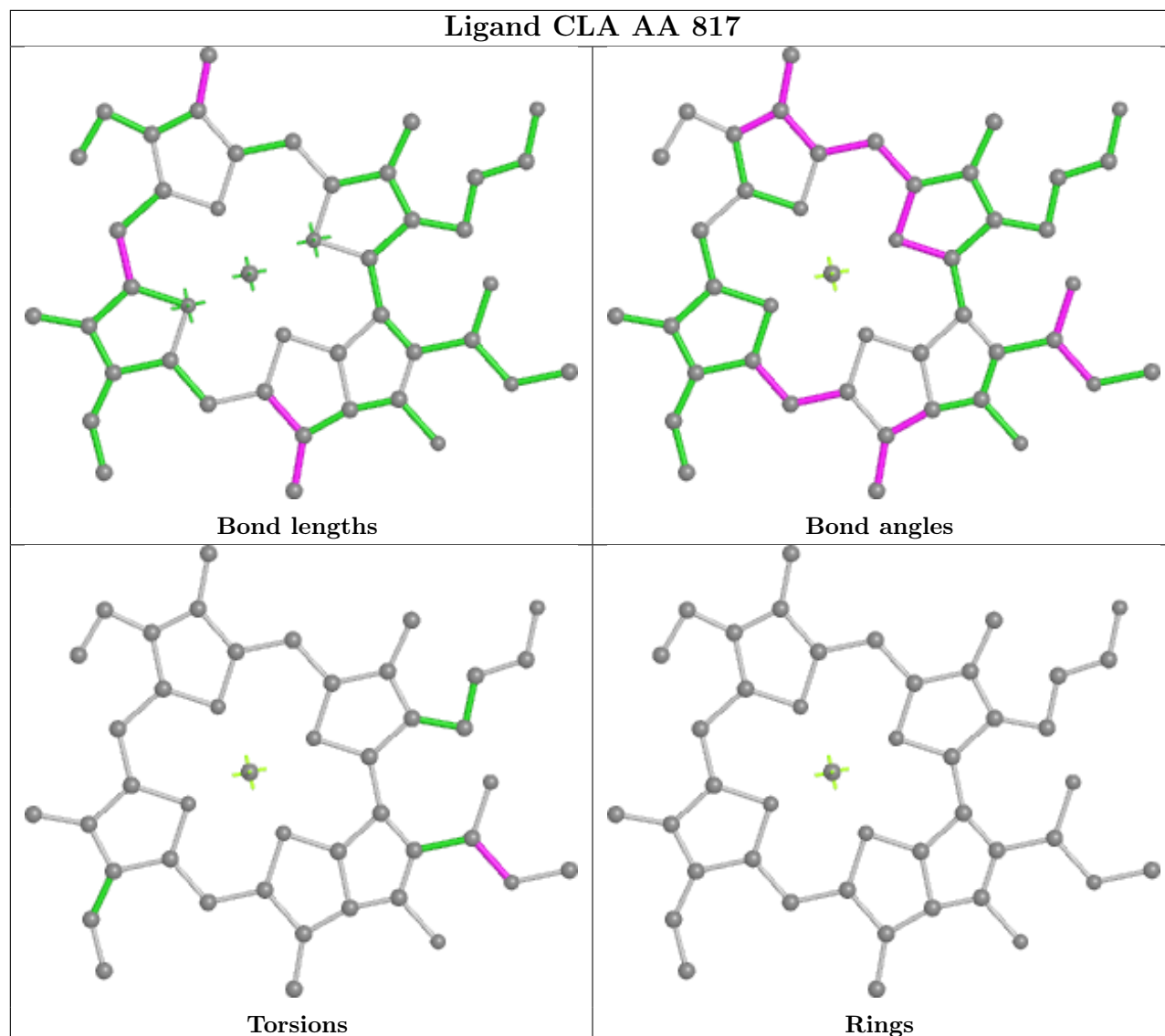
Ligand CLA AA 815



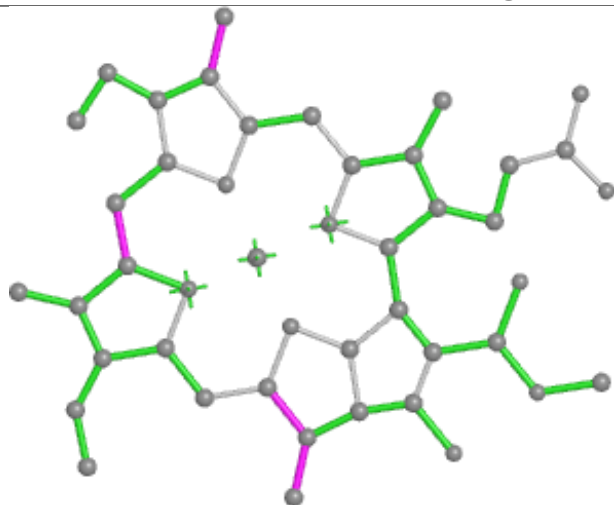
Ligand CLA AA 816



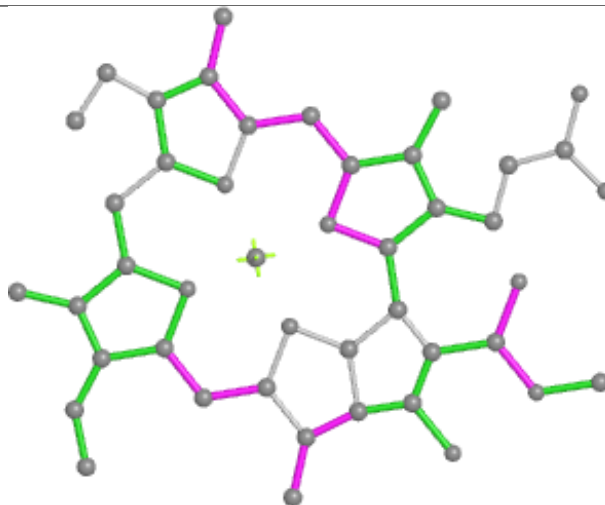
Ligand CLA AA 817



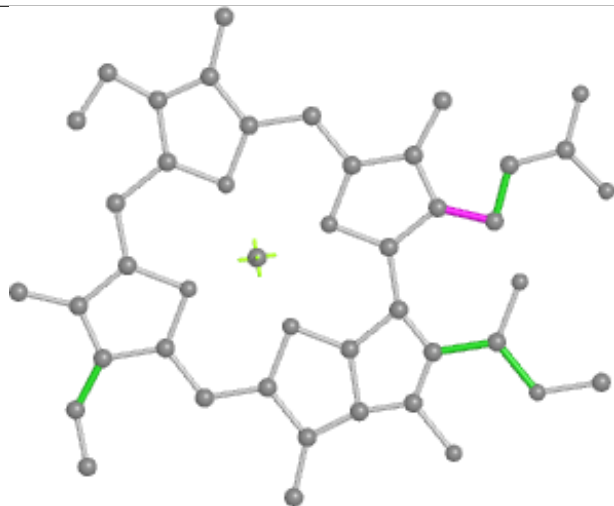
Ligand CLA AA 818



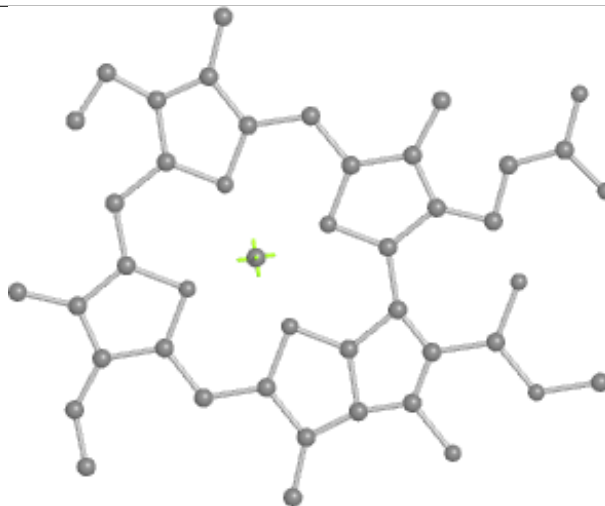
Bond lengths



Bond angles

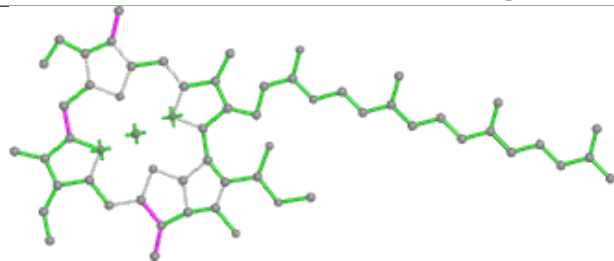


Torsions

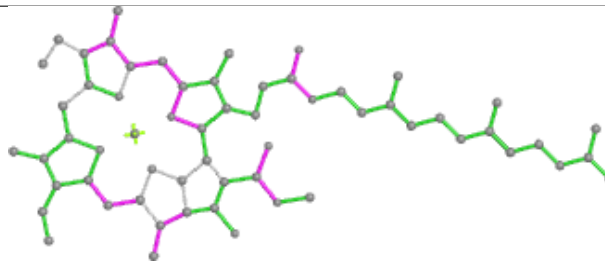


Rings

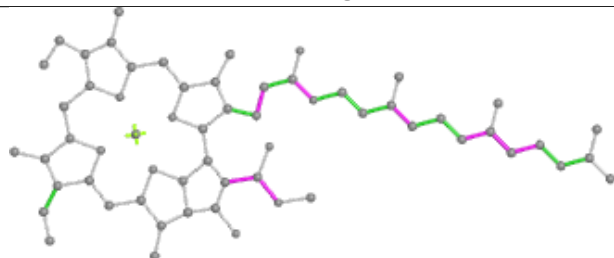
Ligand CLA AA 819



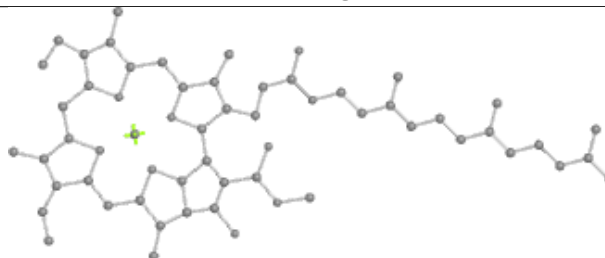
Bond lengths



Bond angles

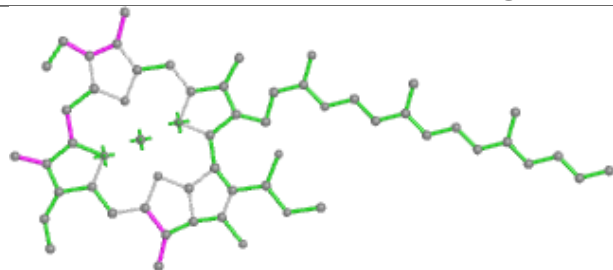


Torsions

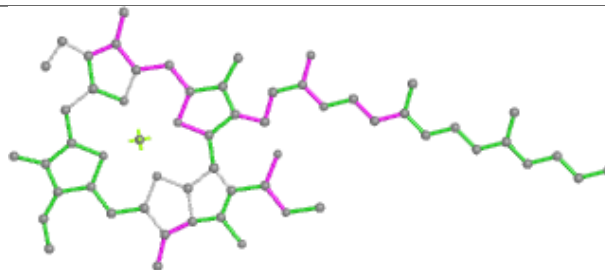


Rings

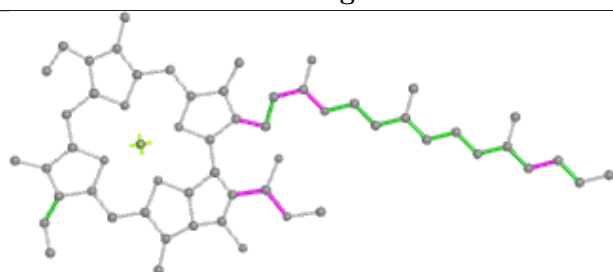
Ligand CLA AA 820



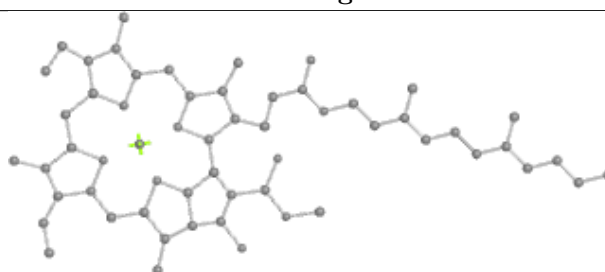
Bond lengths



Bond angles

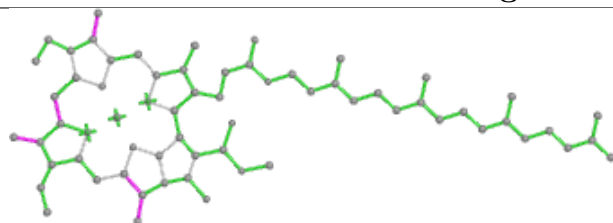


Torsions

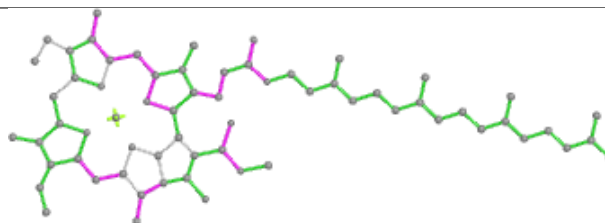


Rings

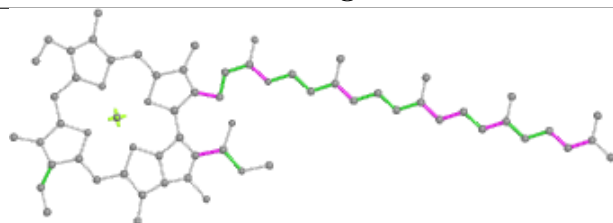
Ligand CLA AA 821



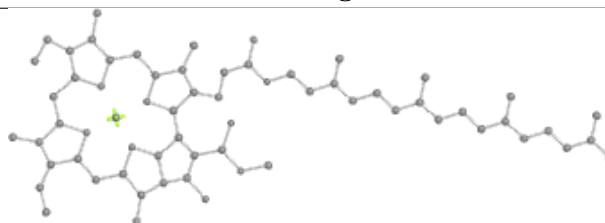
Bond lengths



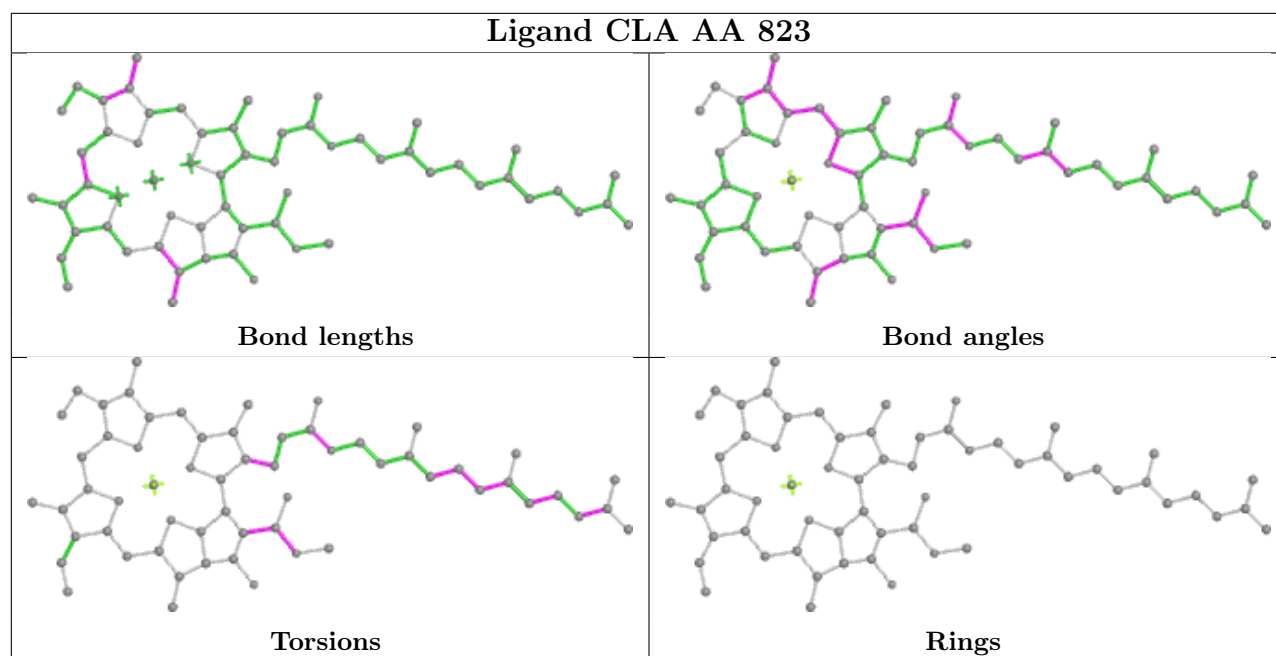
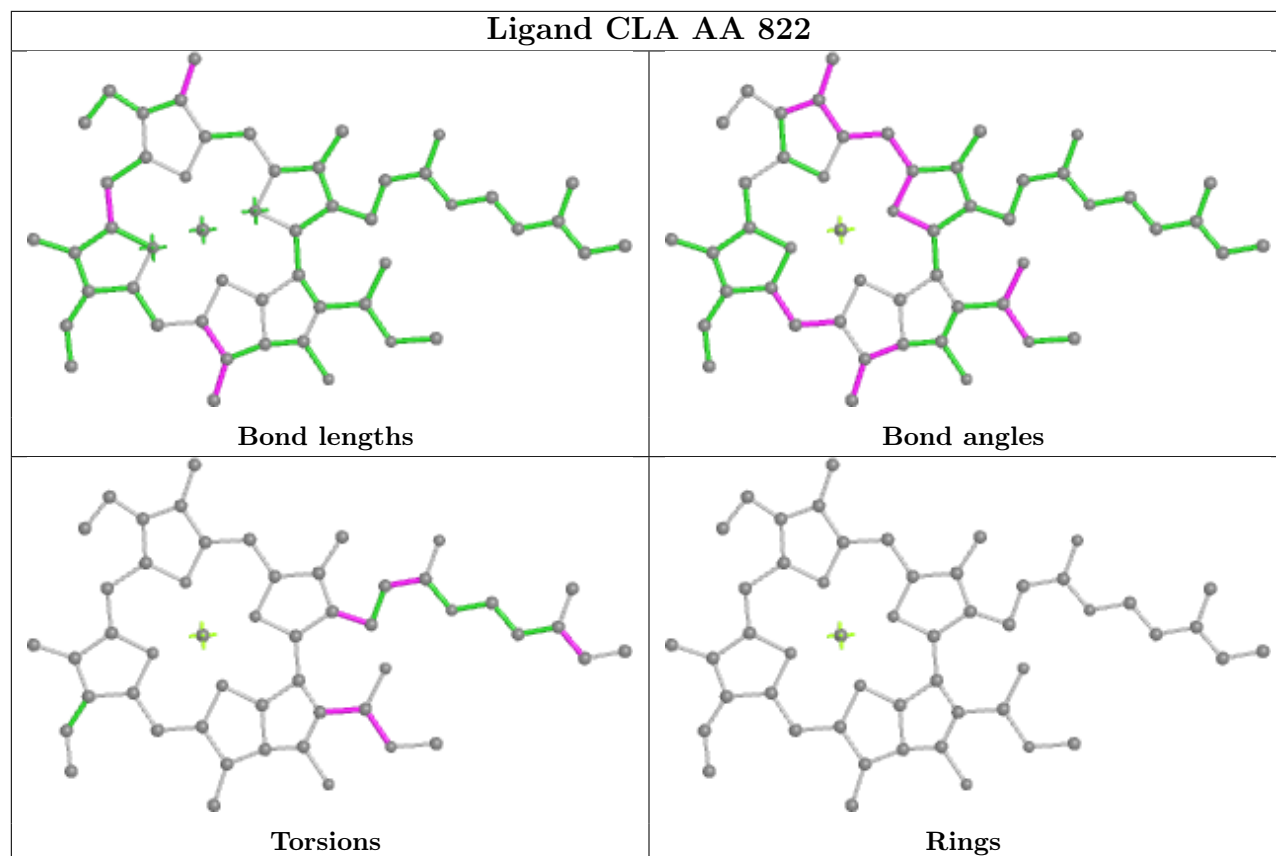
Bond angles



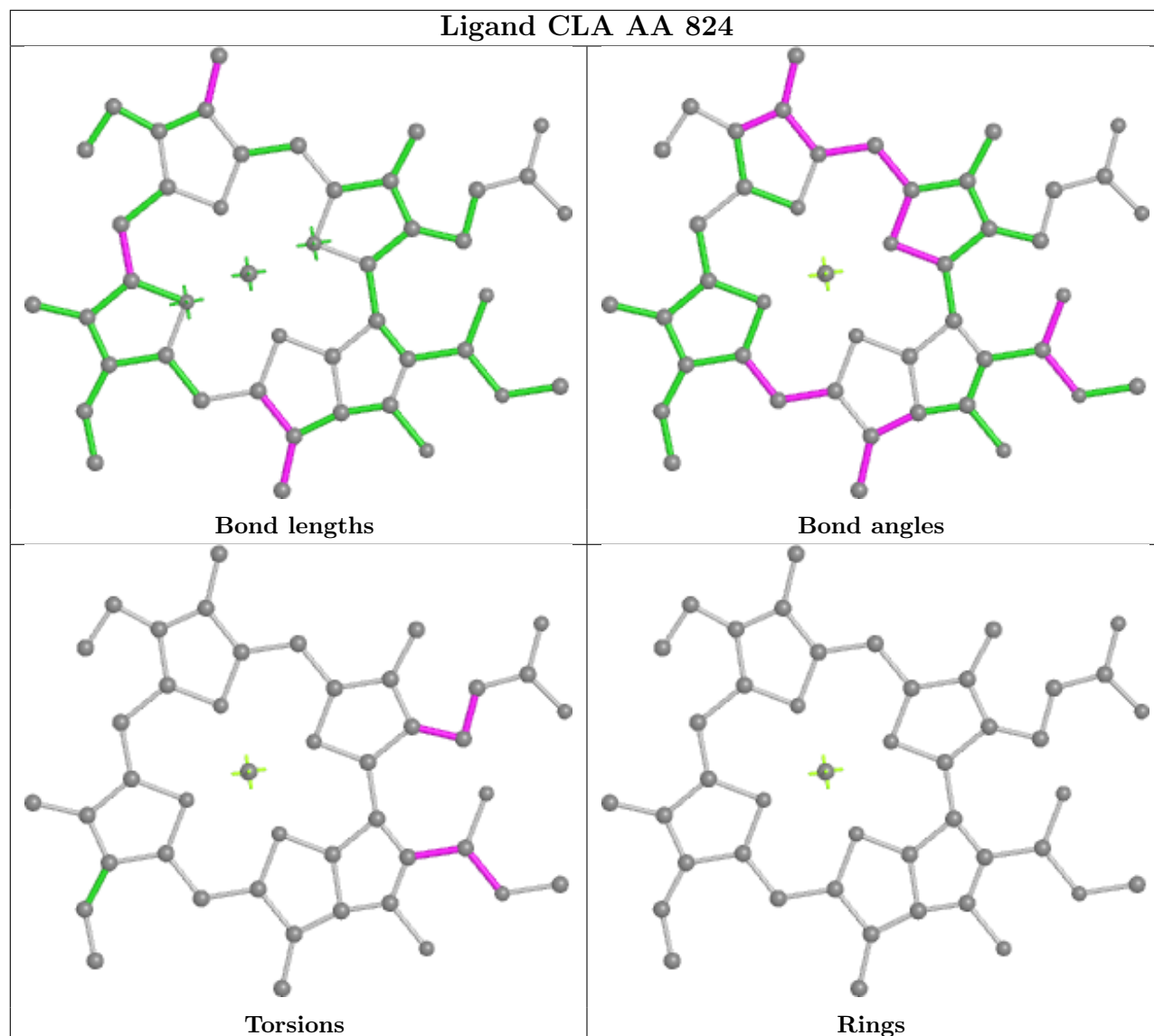
Torsions

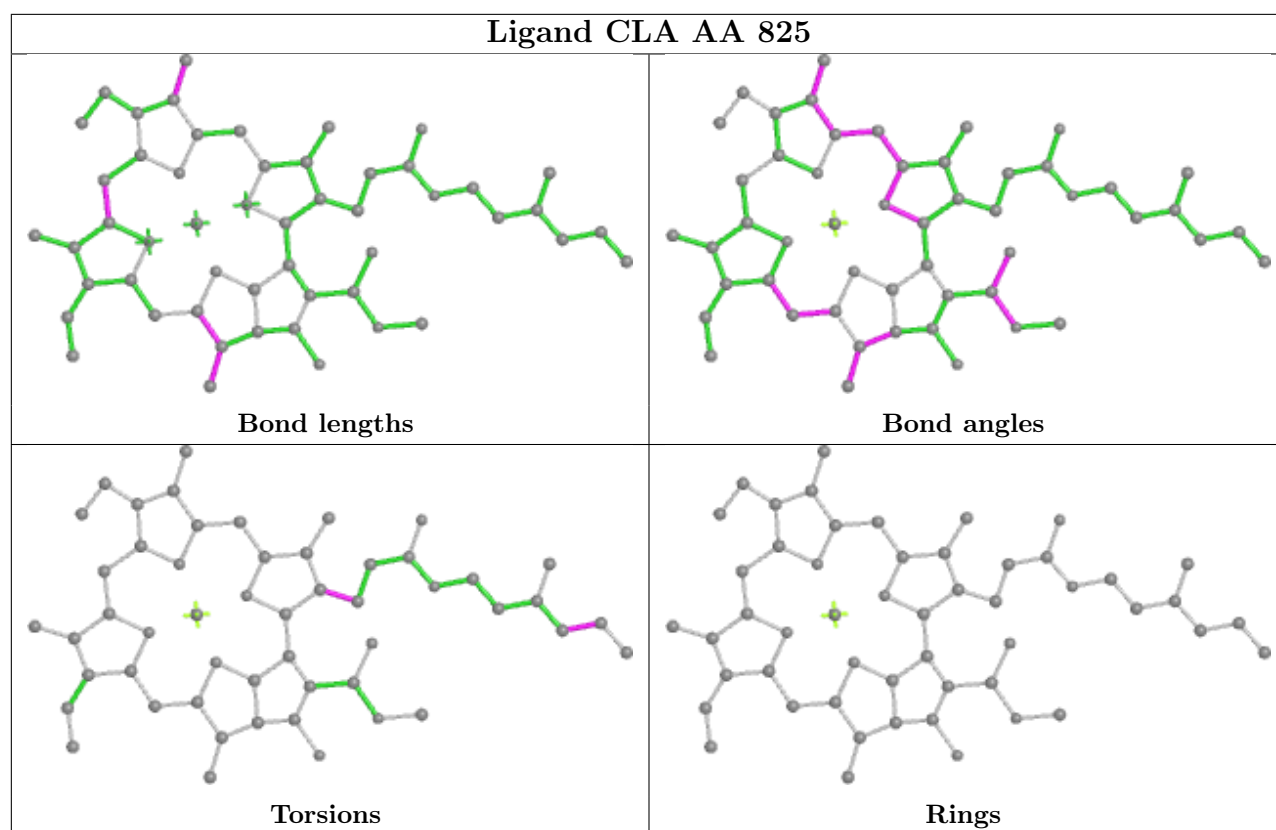


Rings

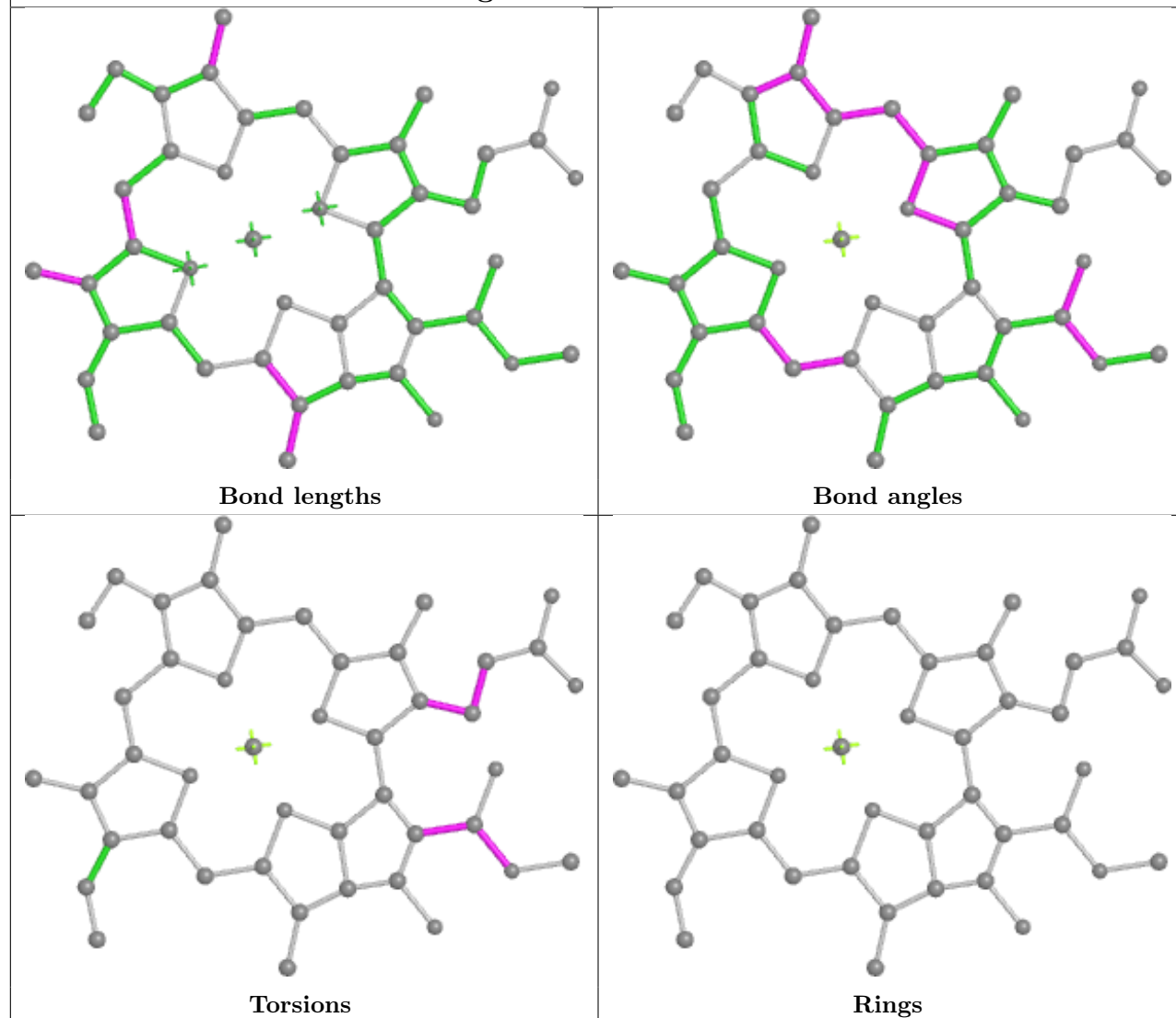


Ligand CLA AA 824

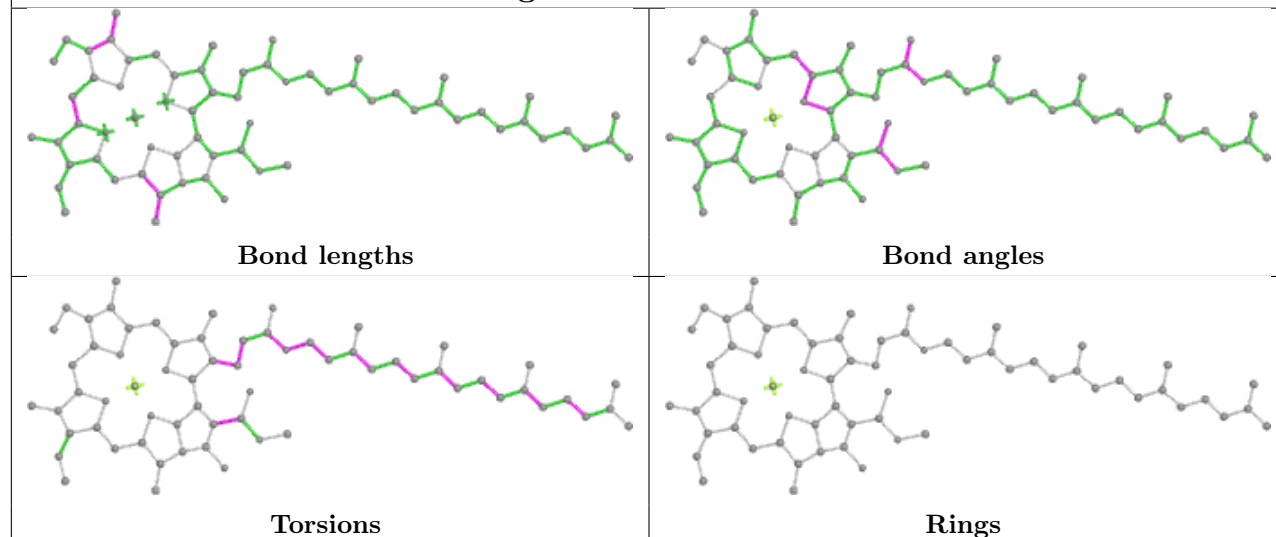




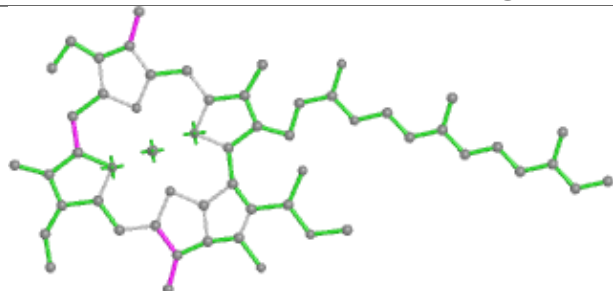
Ligand CLA AA 826



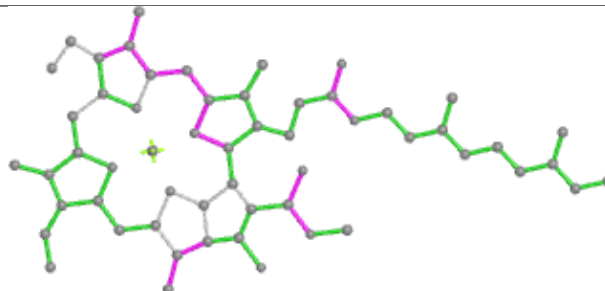
Ligand CLA AA 827



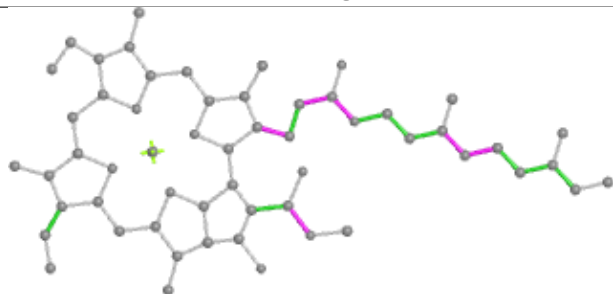
Ligand CLA AA 828



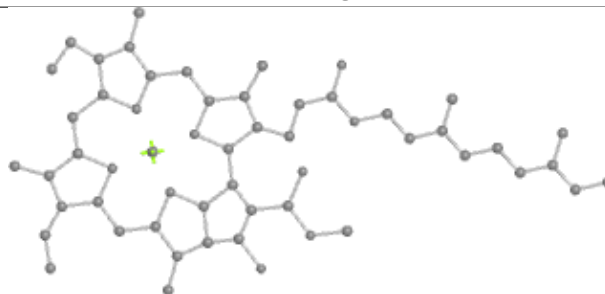
Bond lengths



Bond angles

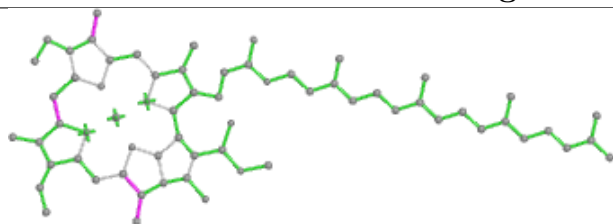


Torsions

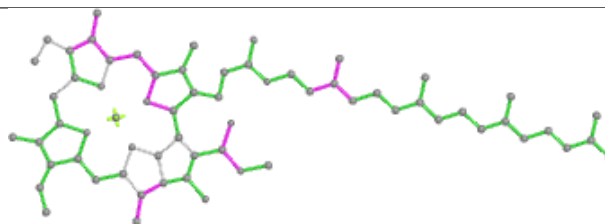


Rings

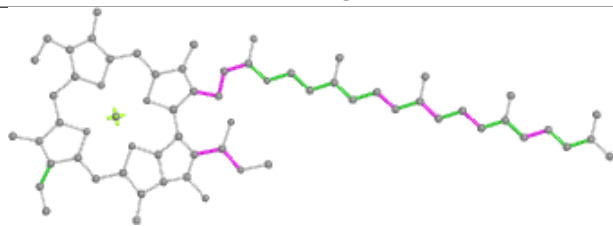
Ligand CLA AA 829



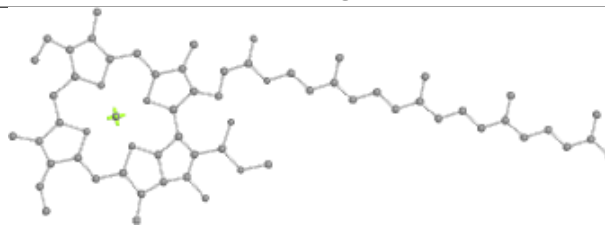
Bond lengths



Bond angles

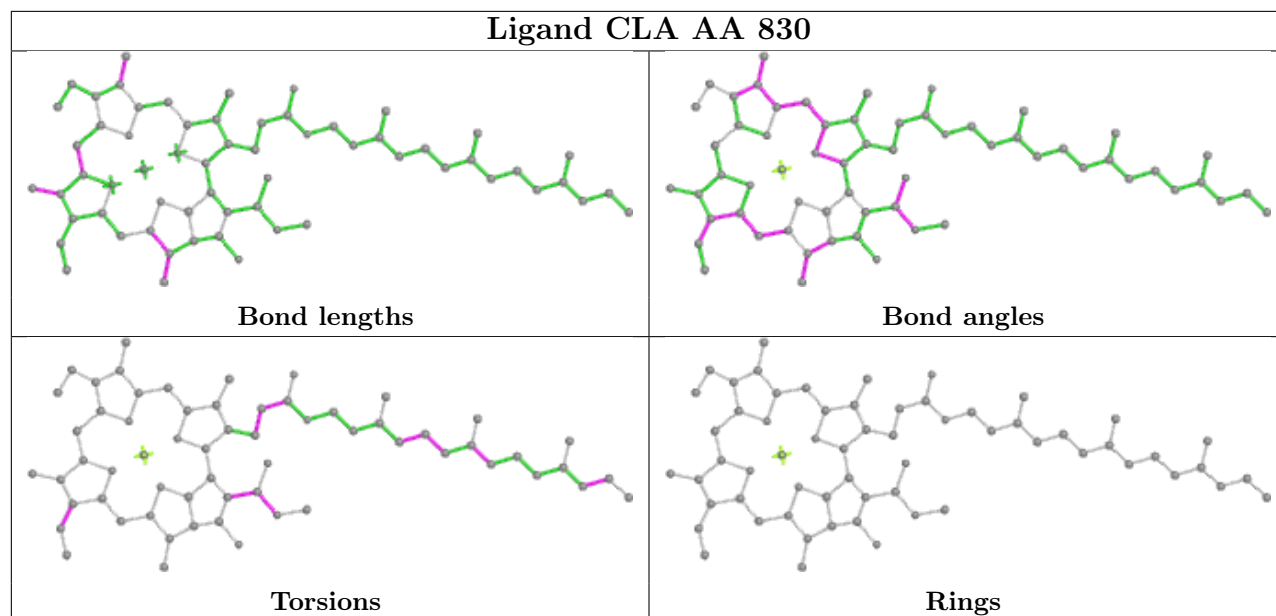


Torsions

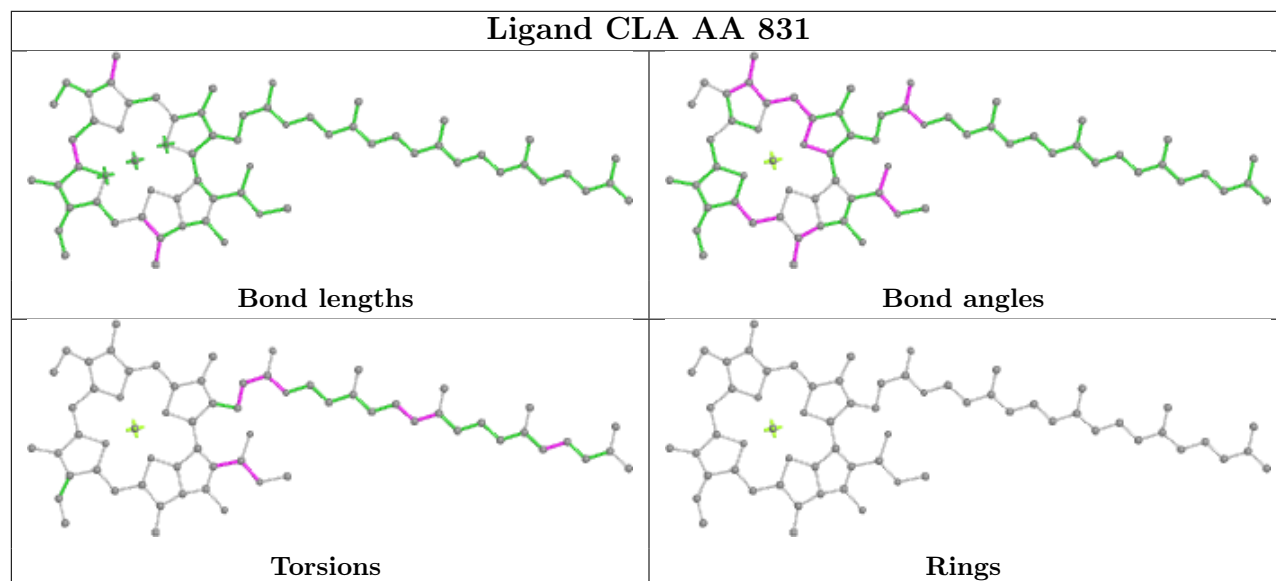


Rings

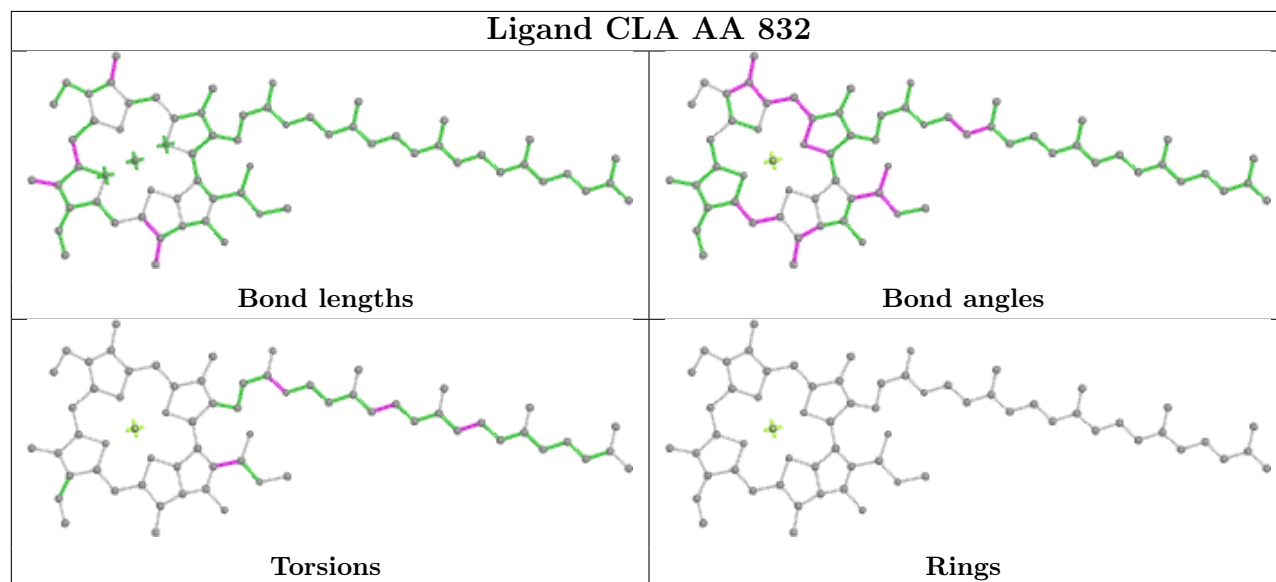
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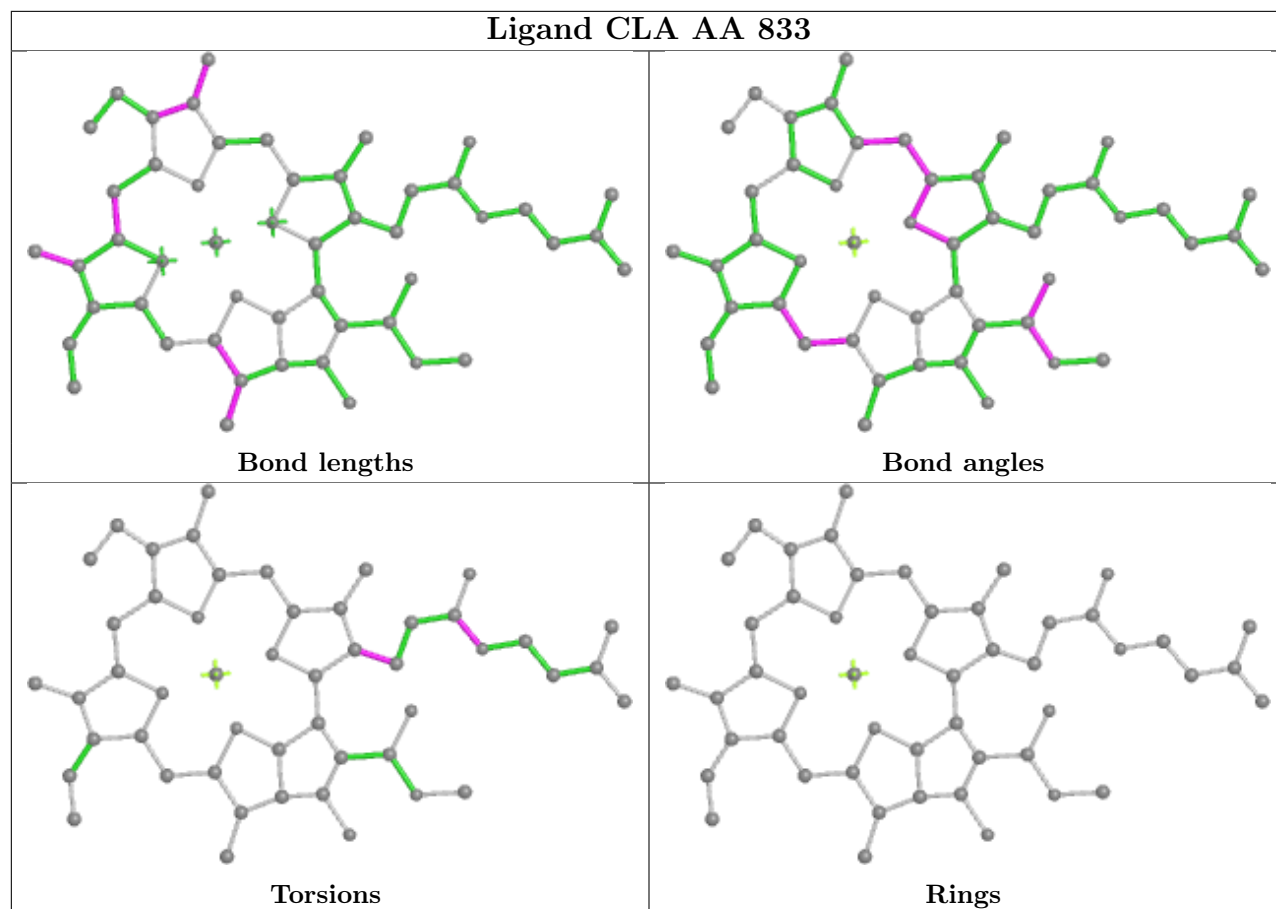
Ligand CLA AA 831



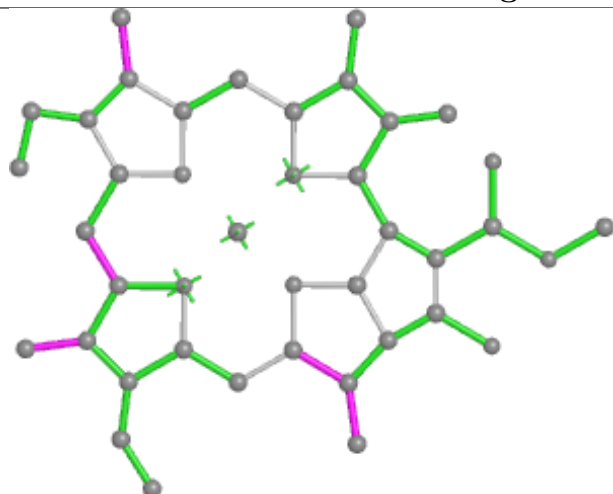
Ligand CLA AA 832



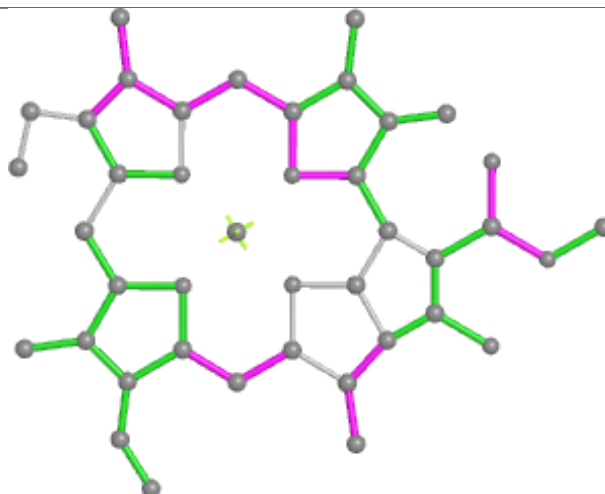
Ligand CLA AA 833



Ligand CLA AA 834



Bond lengths



Bond angles

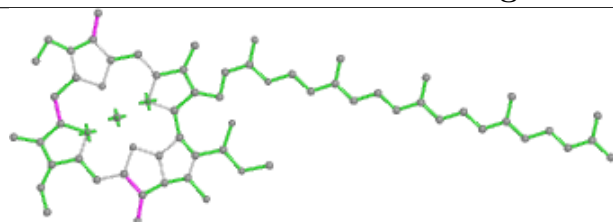


Torsions

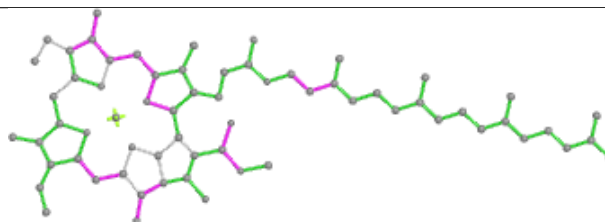


Rings

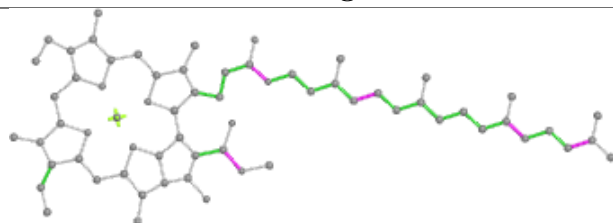
Ligand CLA AA 835



Bond lengths



Bond angles

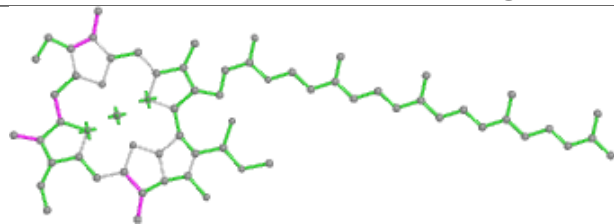


Torsions

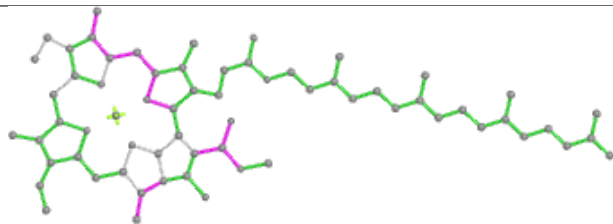


Rings

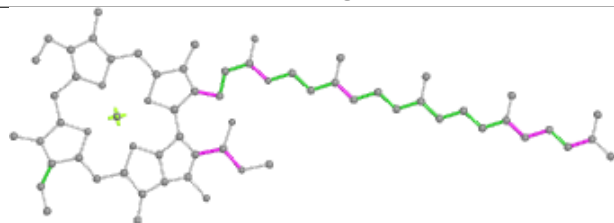
Ligand CLA AA 836



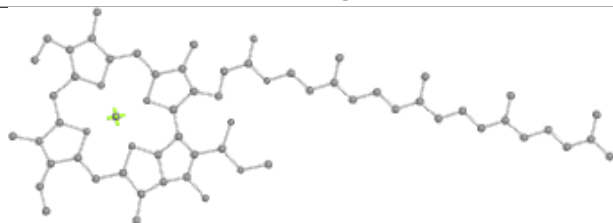
Bond lengths



Bond angles

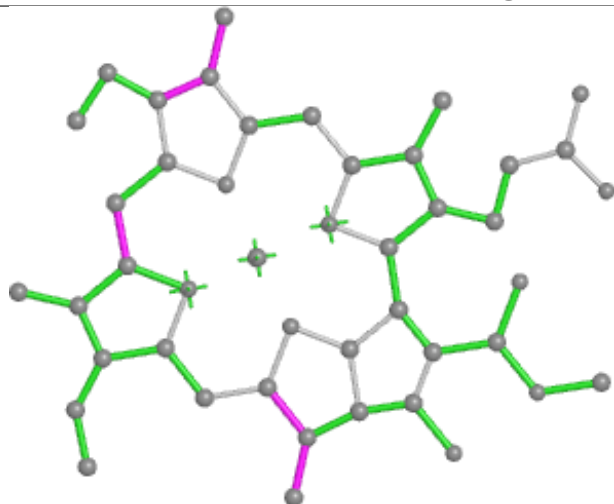


Torsions

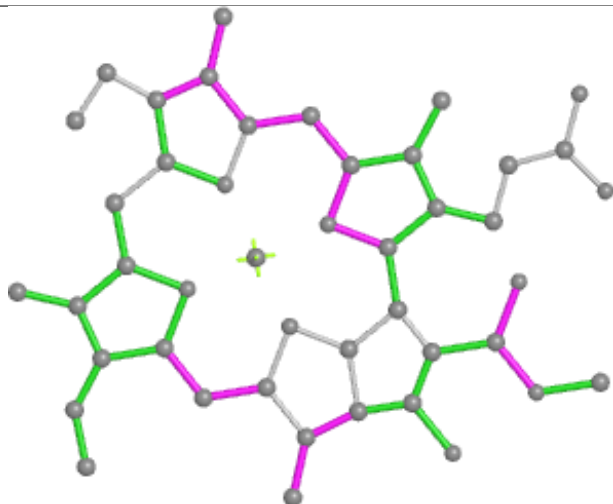


Rings

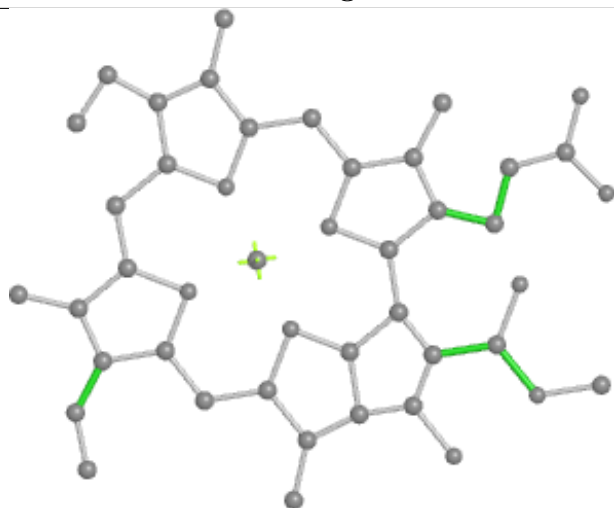
Ligand CLA AA 837



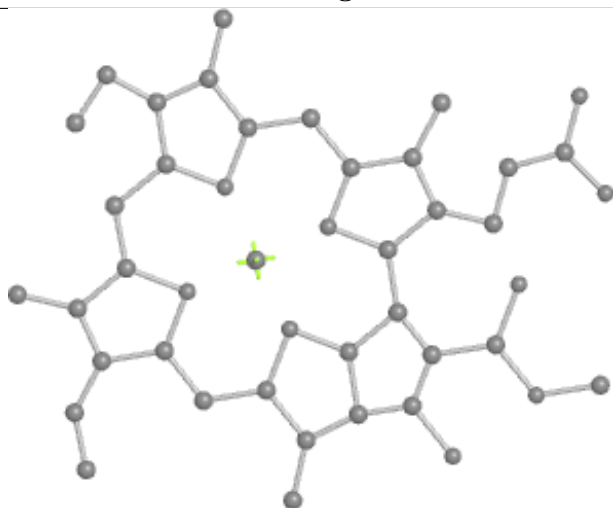
Bond lengths



Bond angles

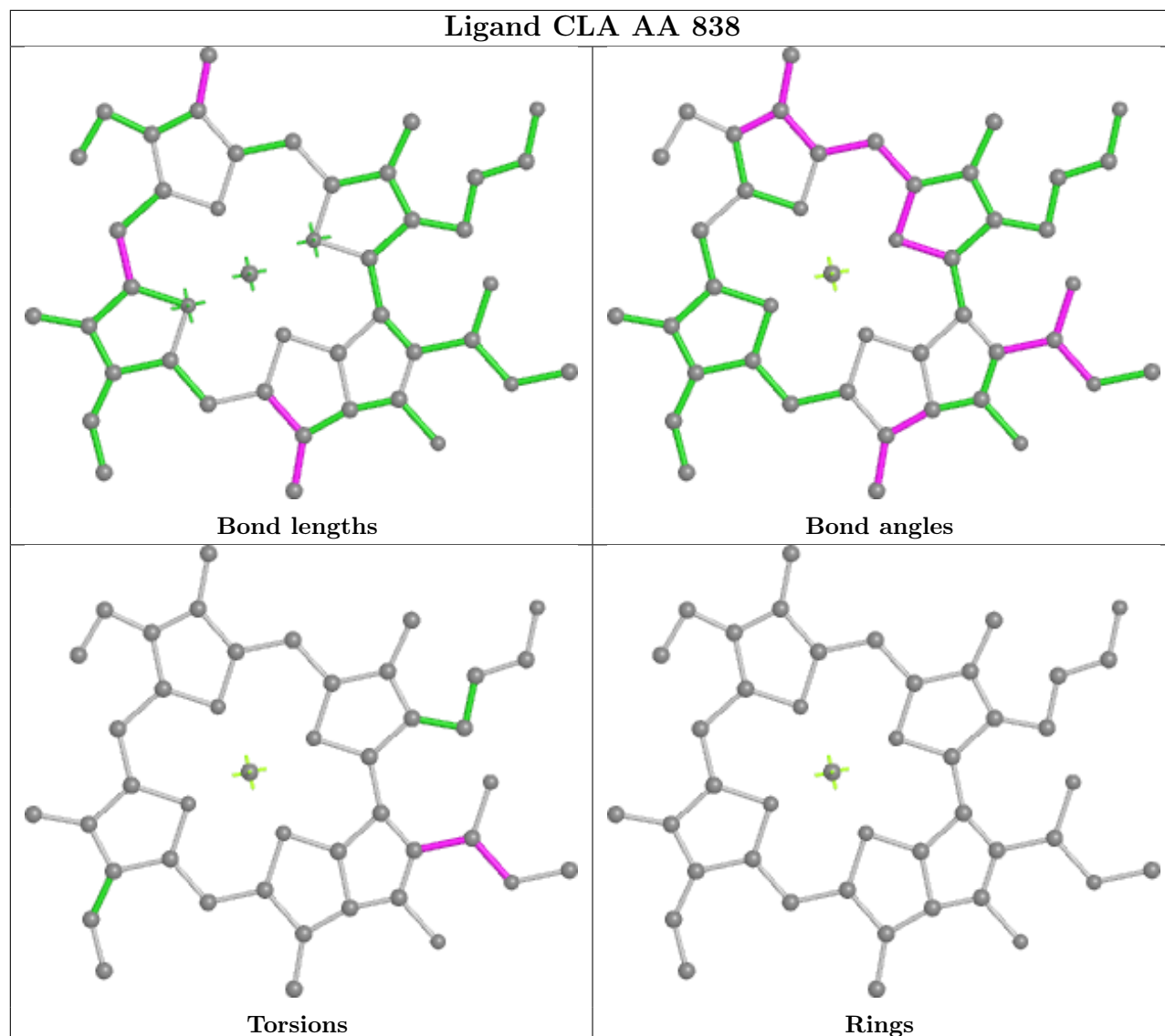


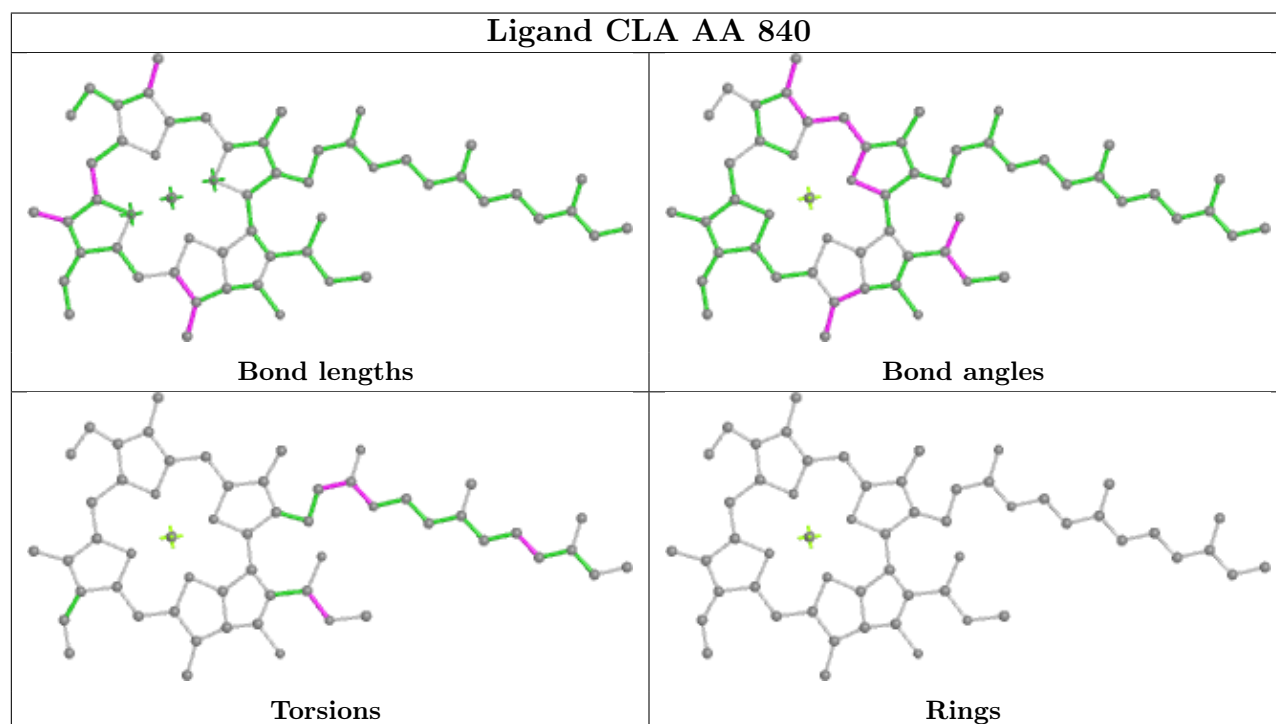
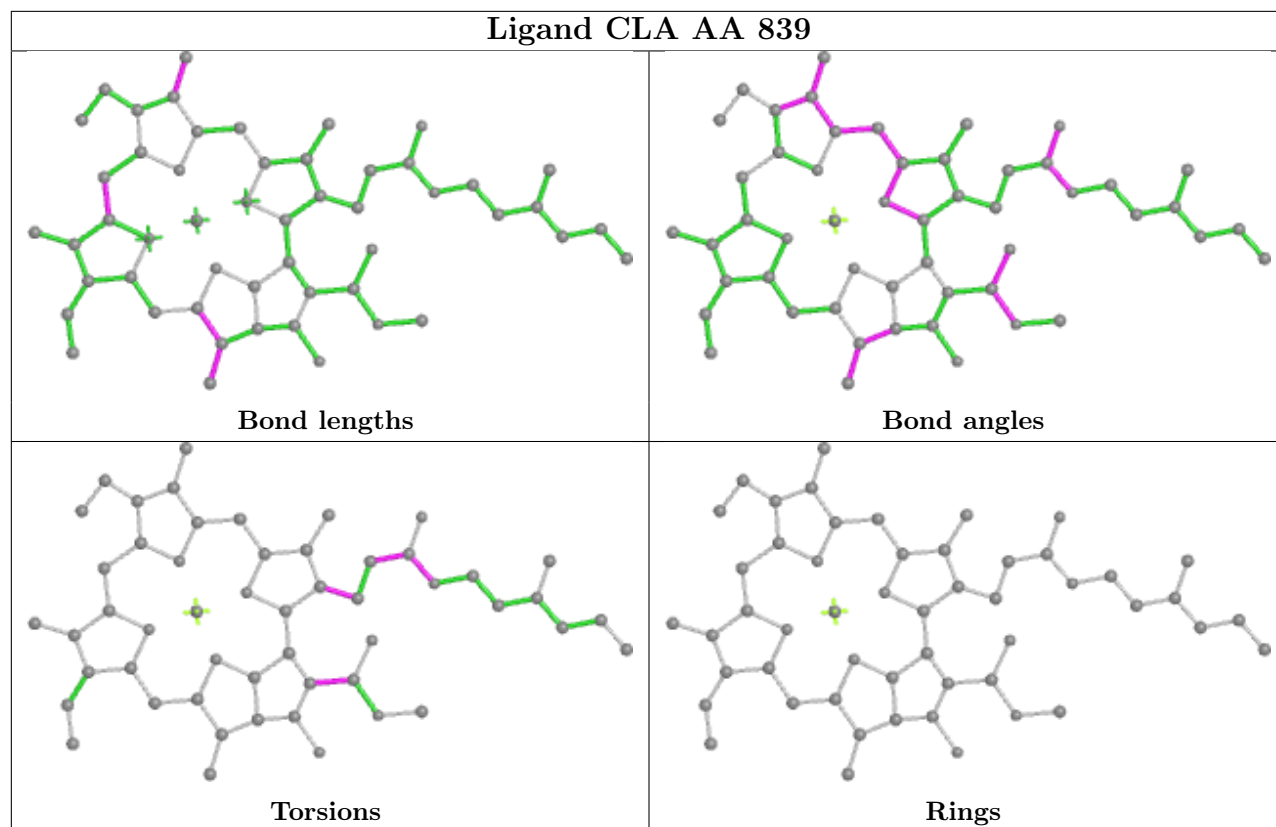
Torsions



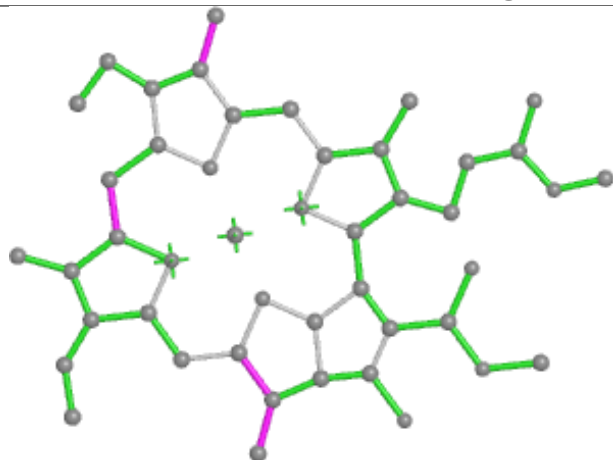
Rings

Ligand CLA AA 838

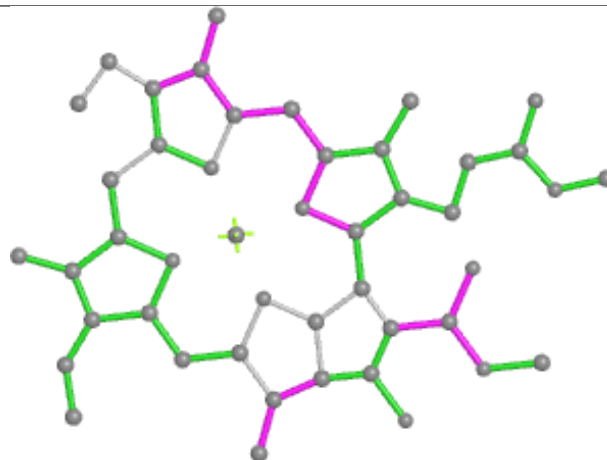




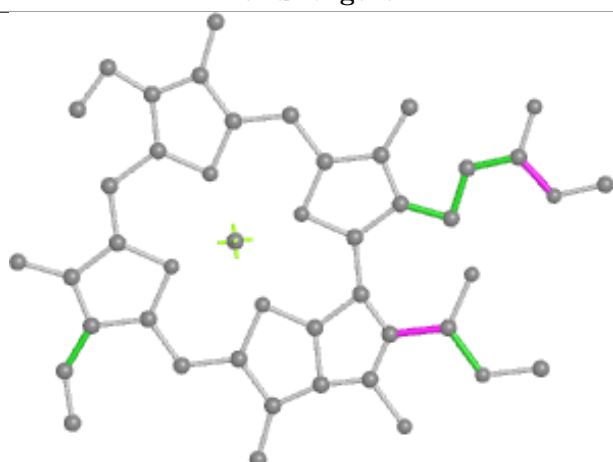
Ligand CLA AA 841



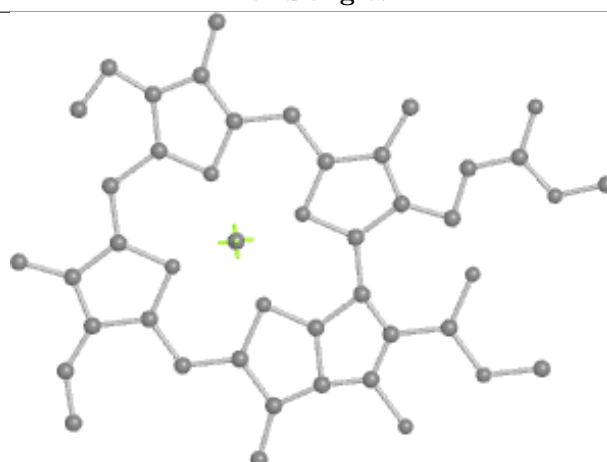
Bond lengths



Bond angles

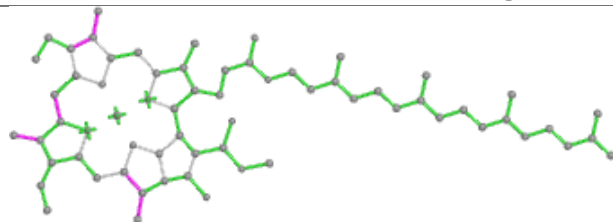


Torsions

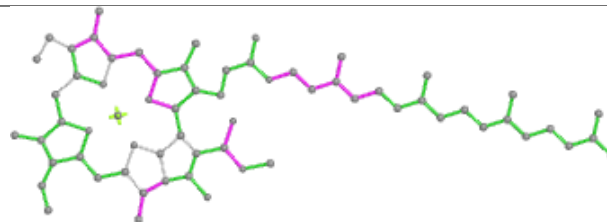


Rings

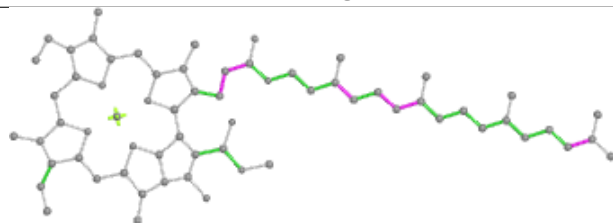
Ligand CLA AA 842



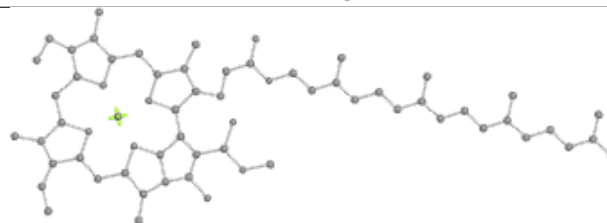
Bond lengths



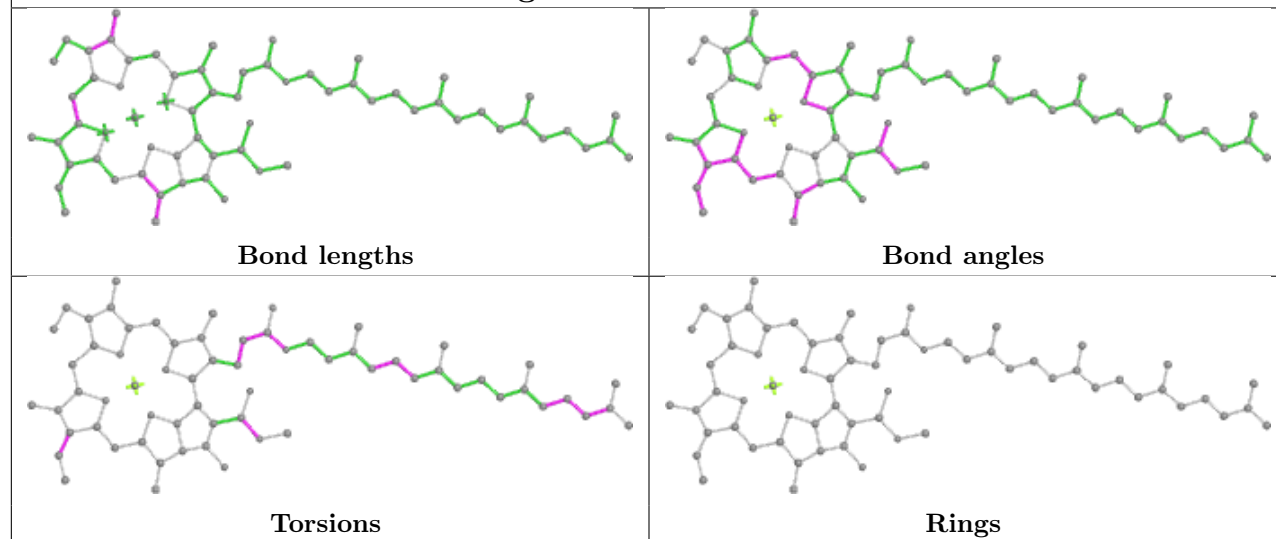
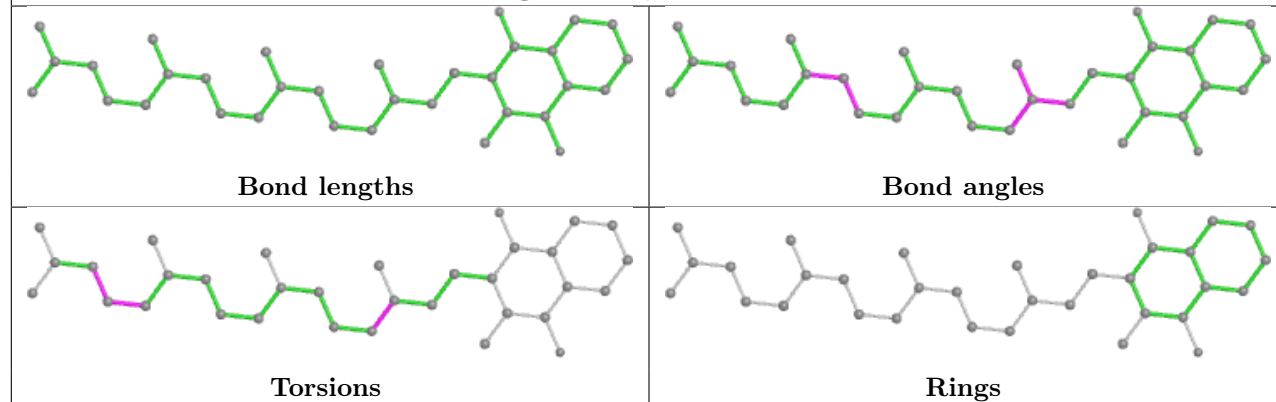
Bond angles



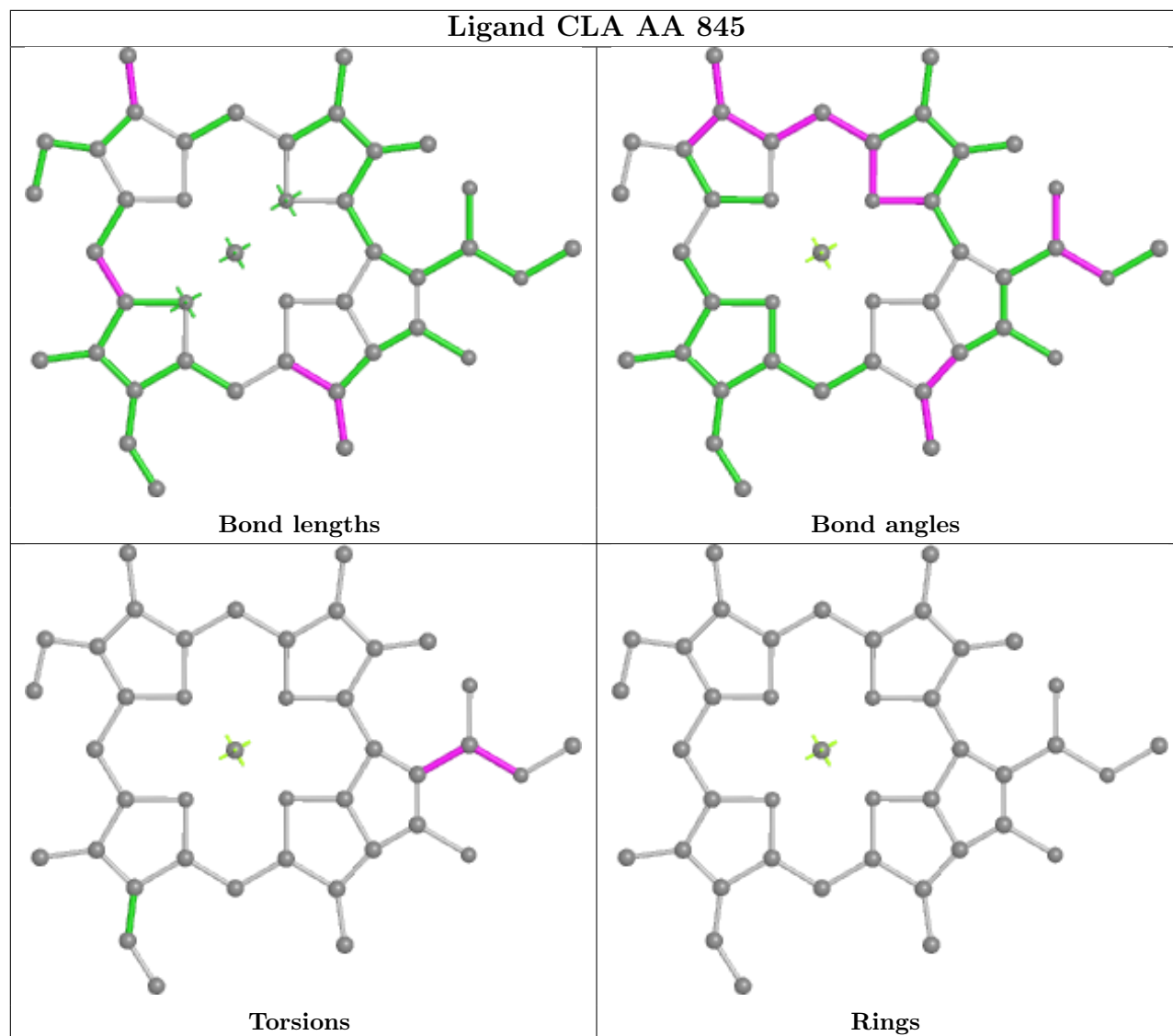
Torsions

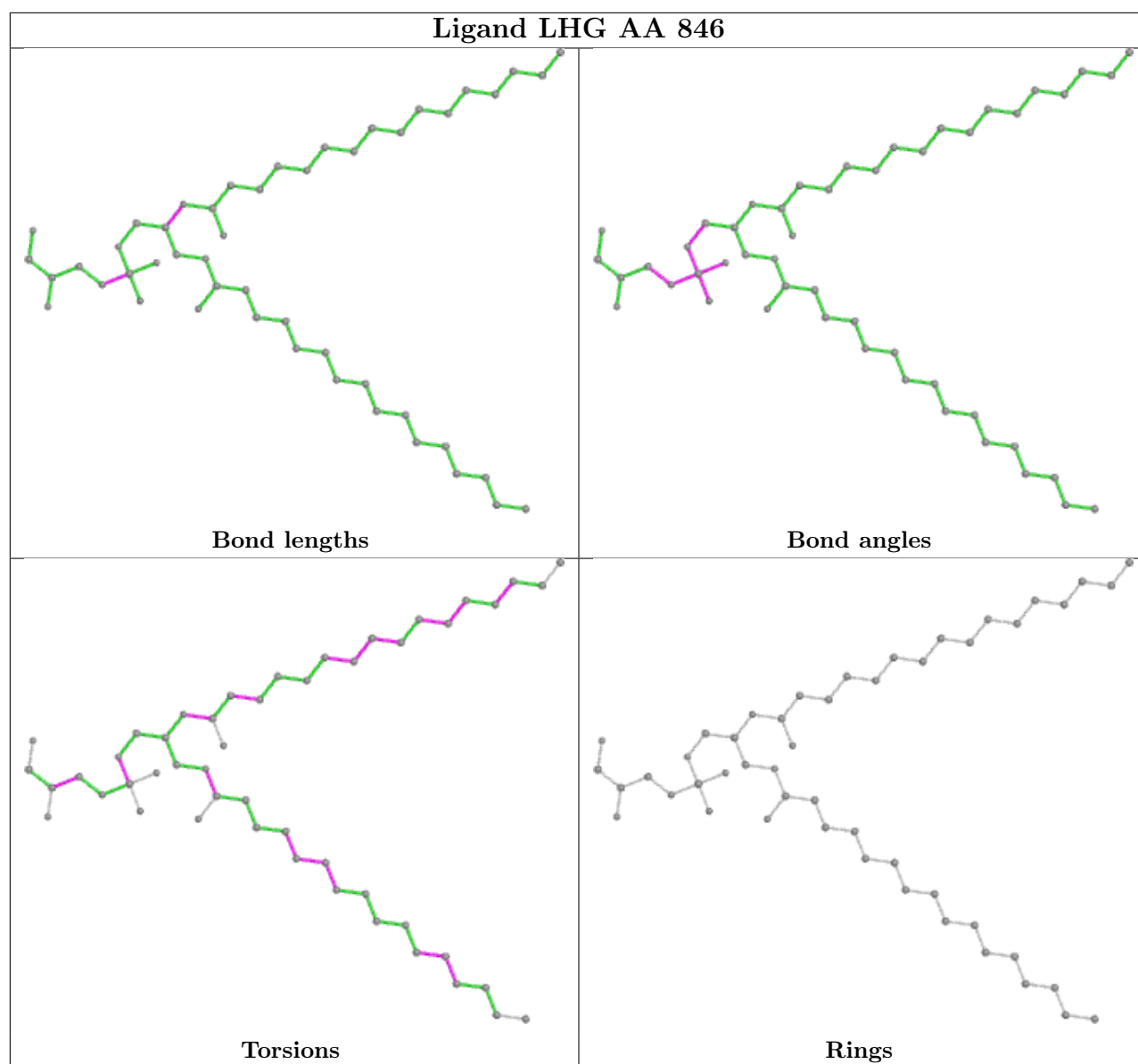


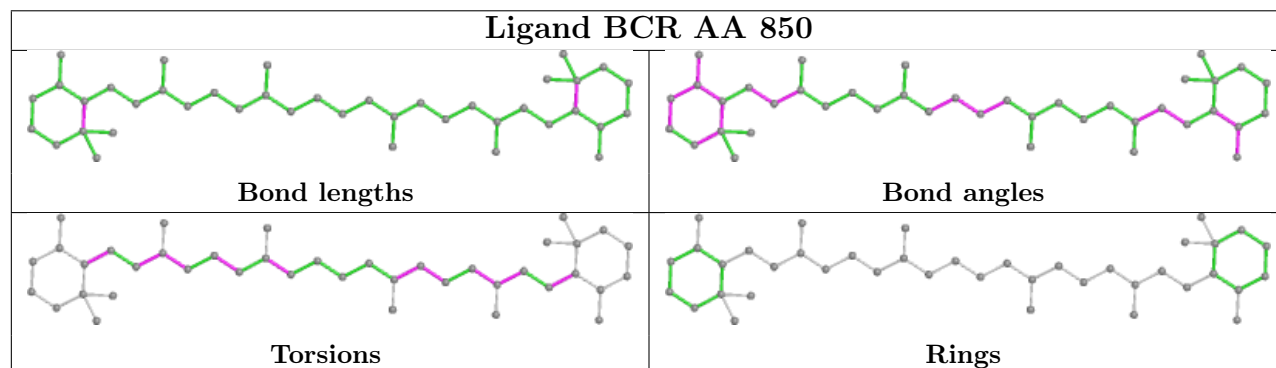
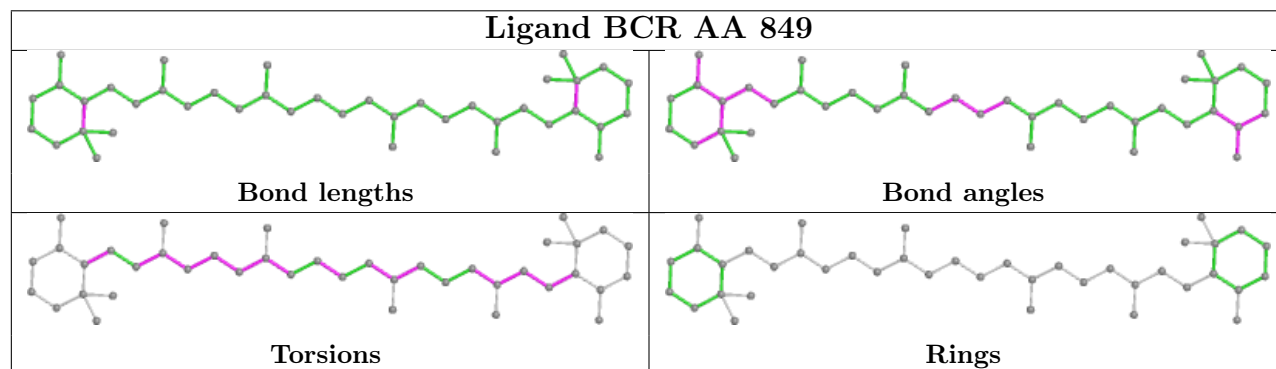
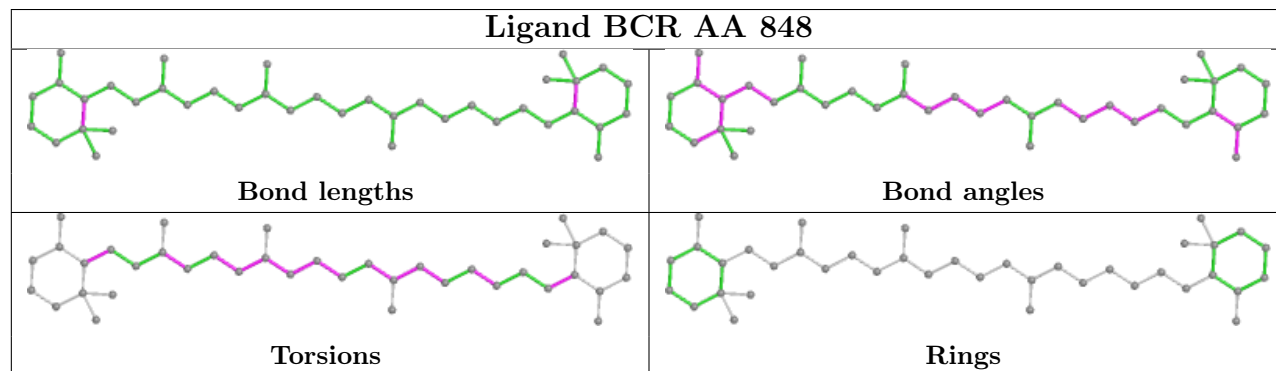
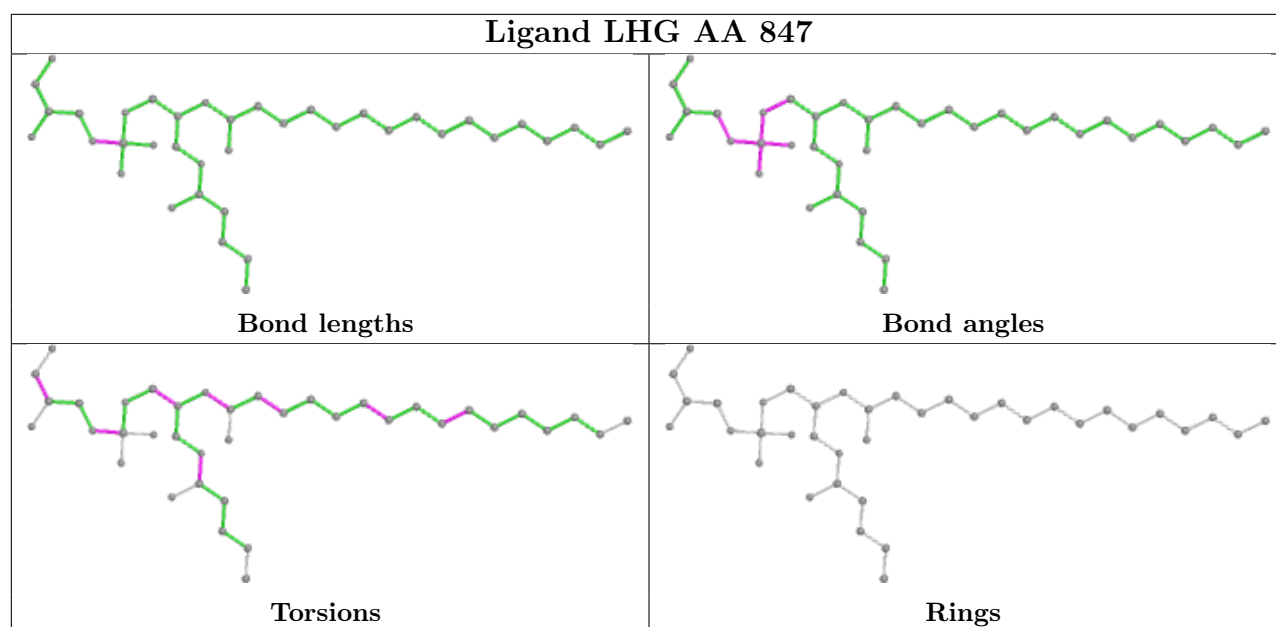
Rings

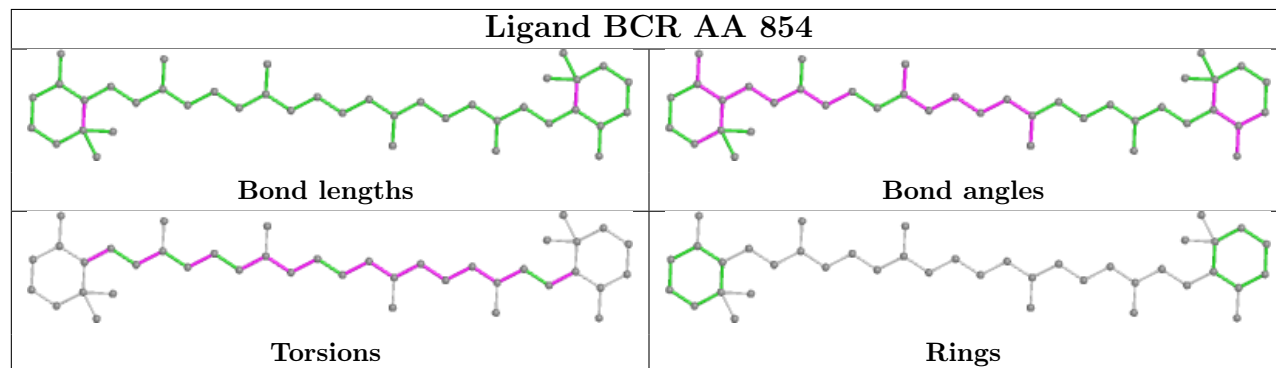
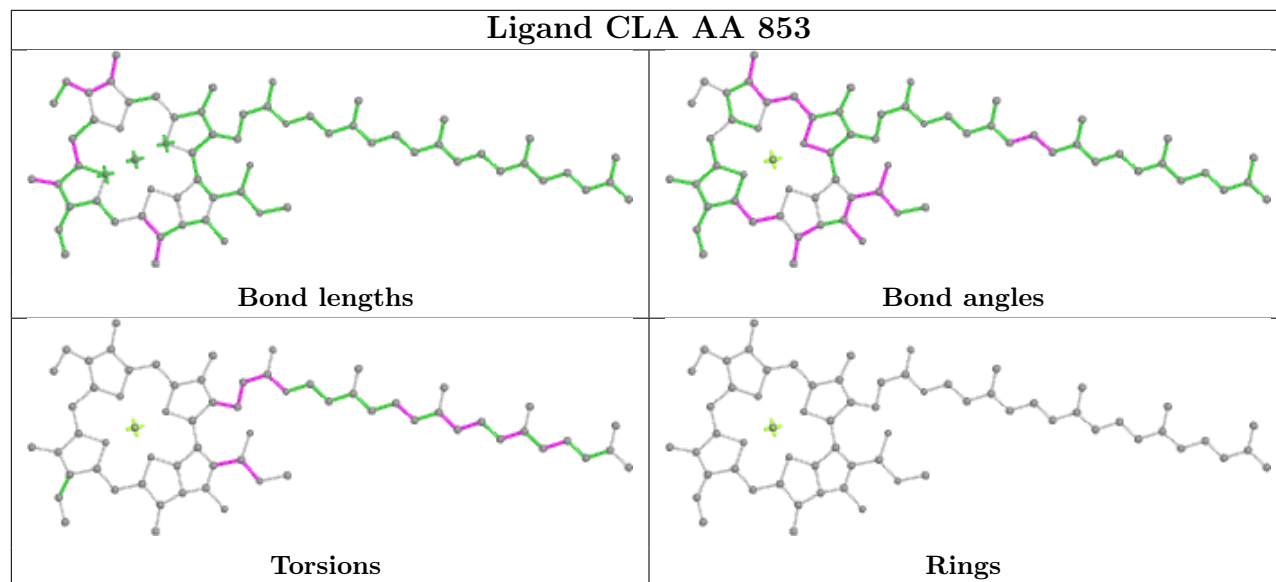
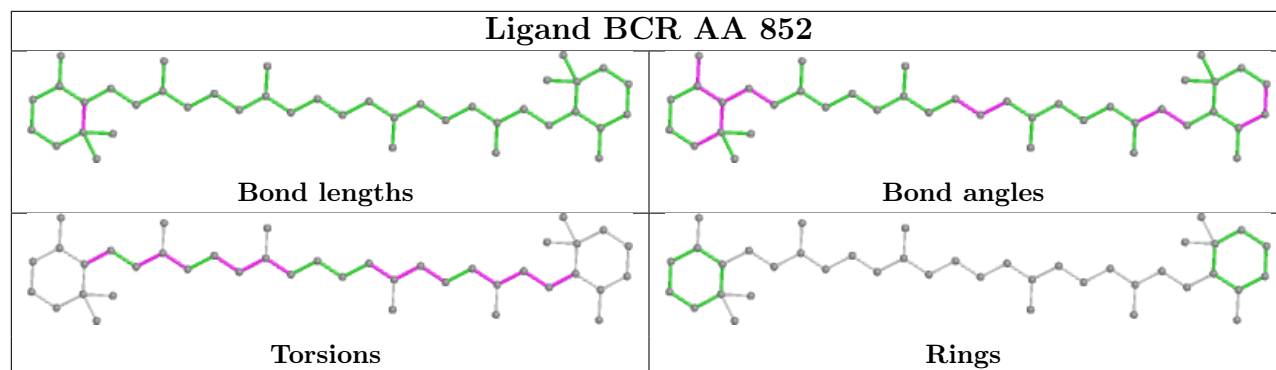
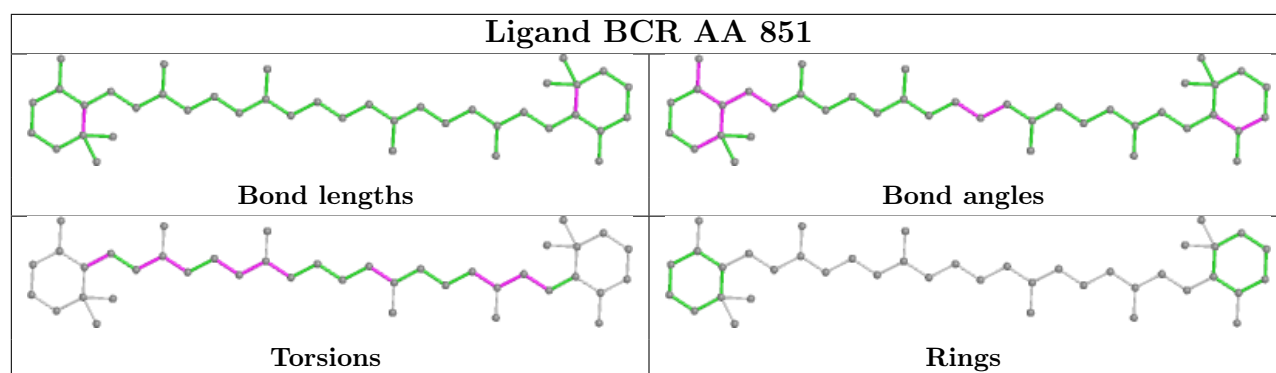
Ligand CLA AA 843**Ligand PQN AA 844**

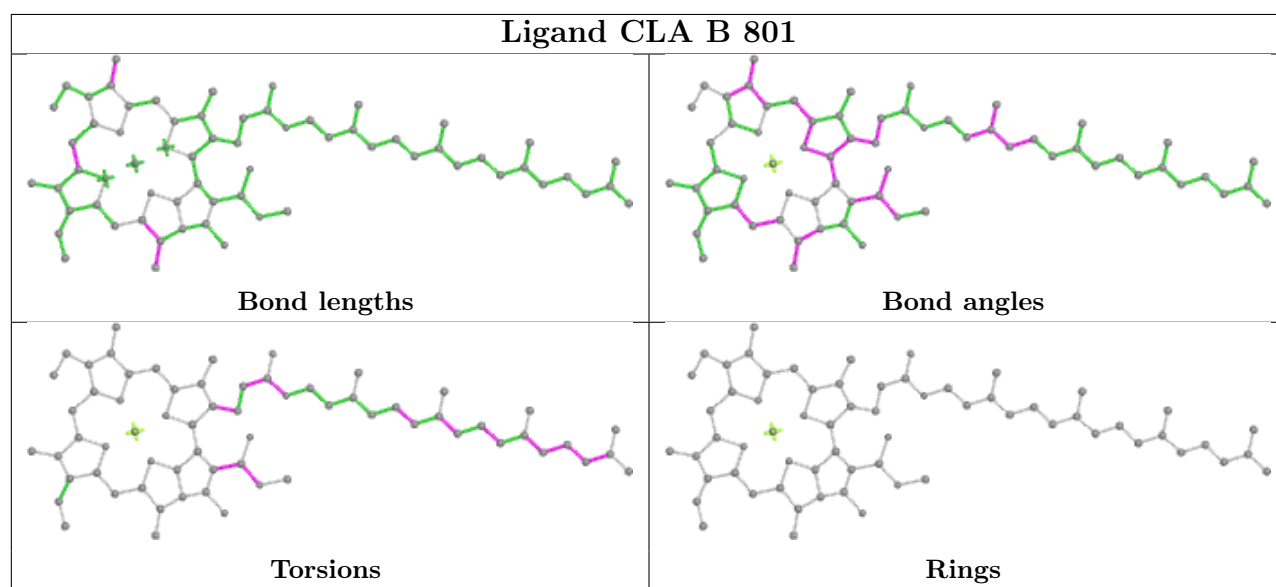
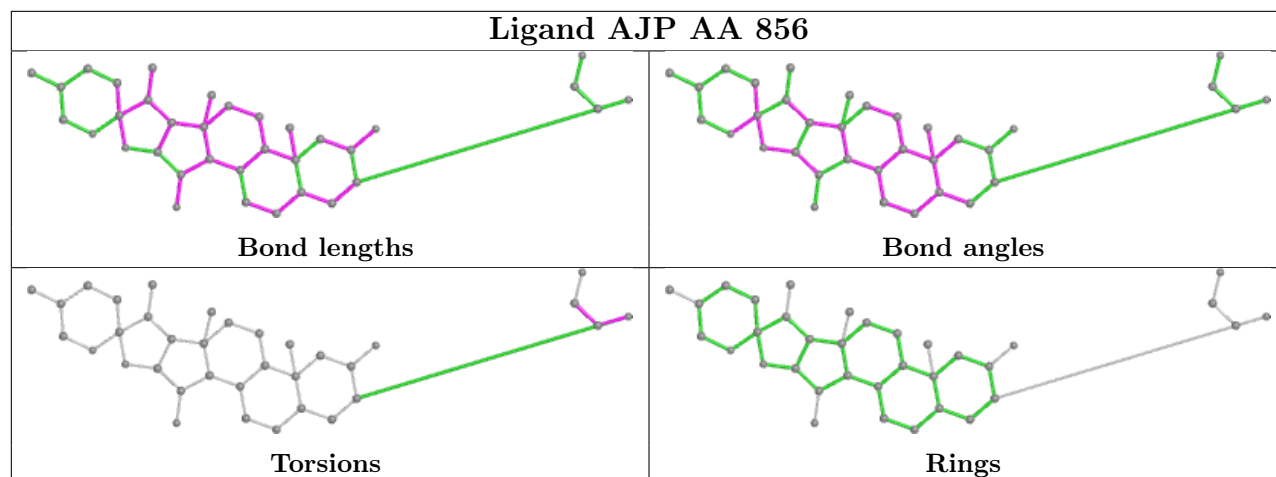
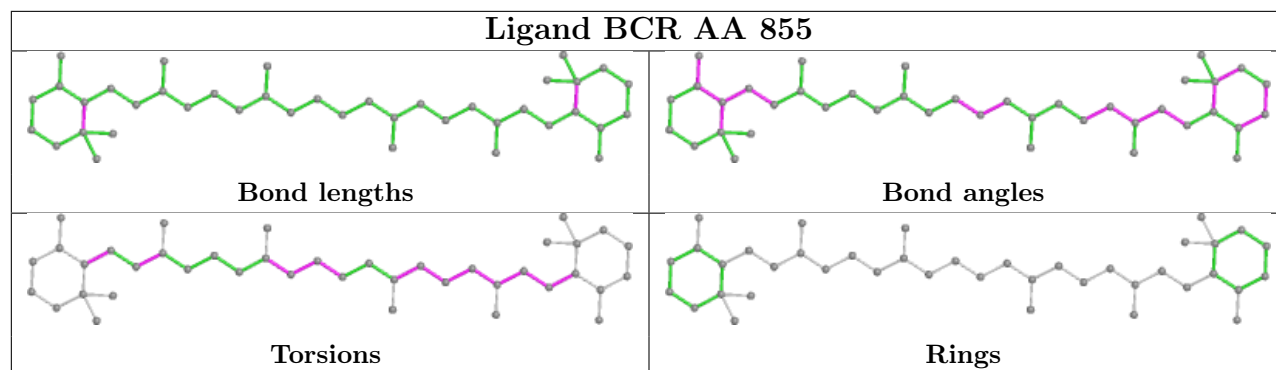
Ligand CLA AA 845



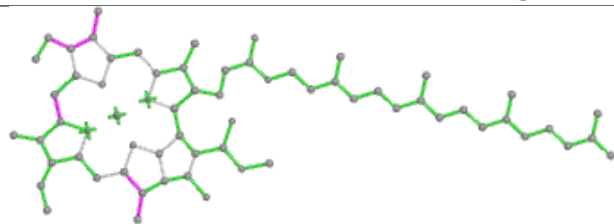




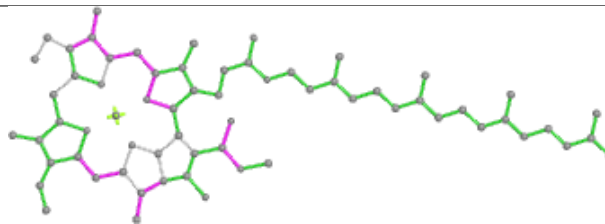




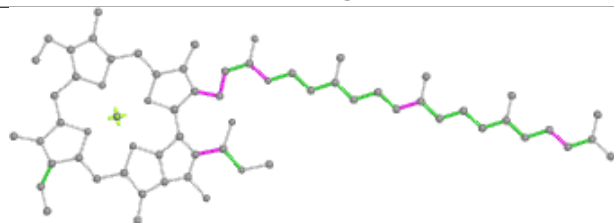
Ligand CLA B 802



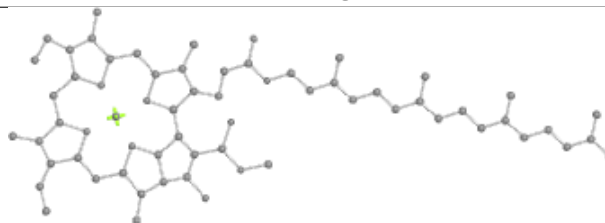
Bond lengths



Bond angles

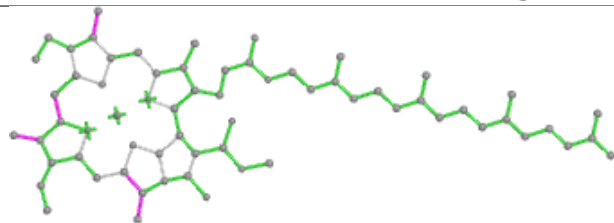


Torsions

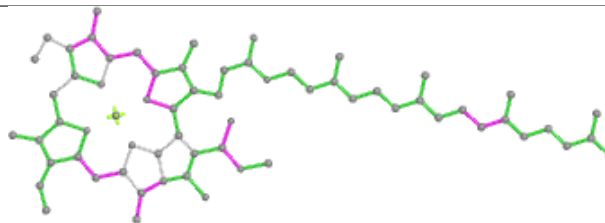


Rings

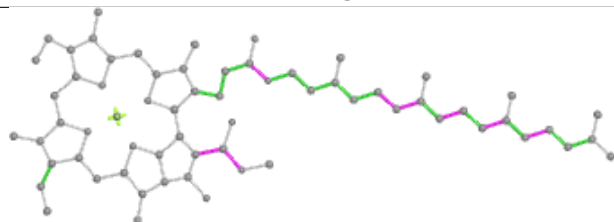
Ligand CLA B 803



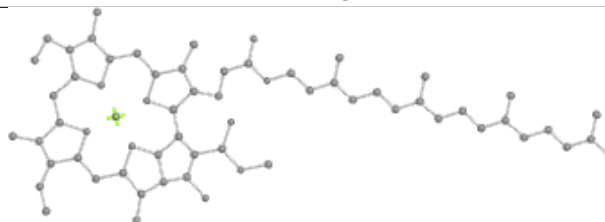
Bond lengths



Bond angles

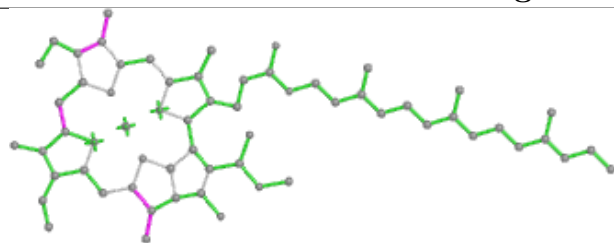


Torsions

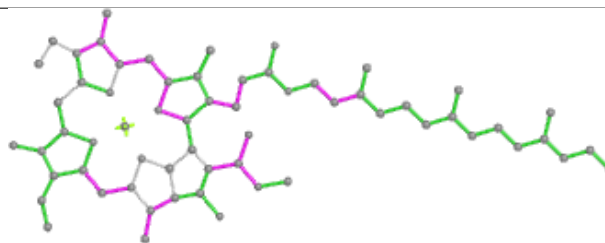


Rings

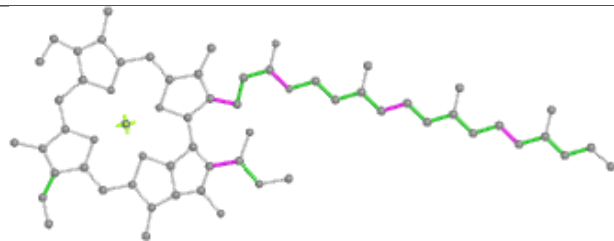
Ligand CLA B 804



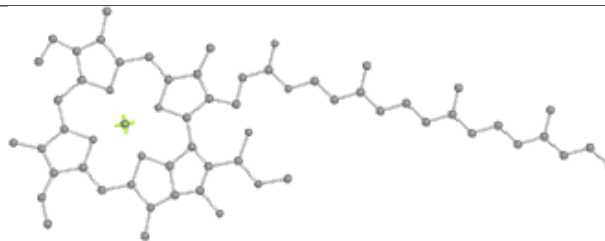
Bond lengths



Bond angles

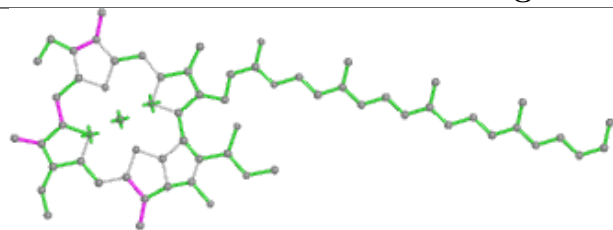


Torsions

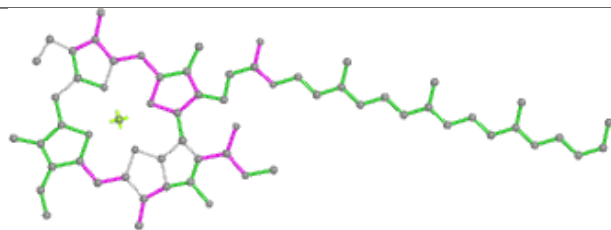


Rings

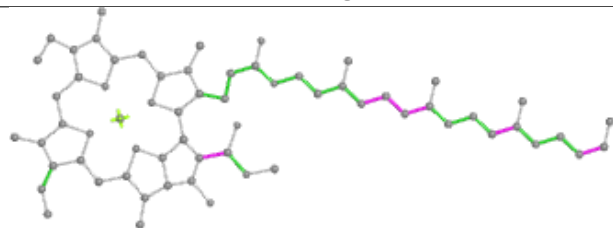
Ligand CLA B 805



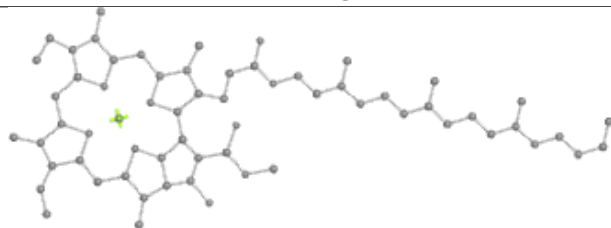
Bond lengths



Bond angles

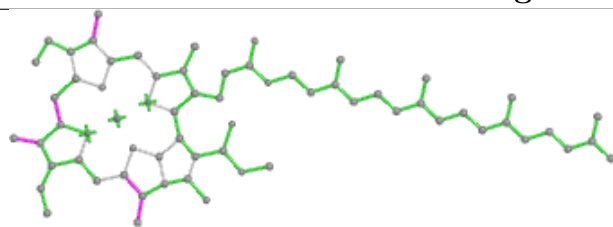


Torsions

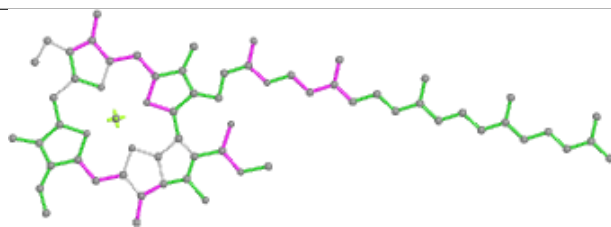


Rings

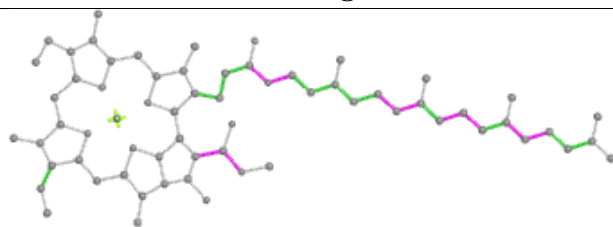
Ligand CLA B 806



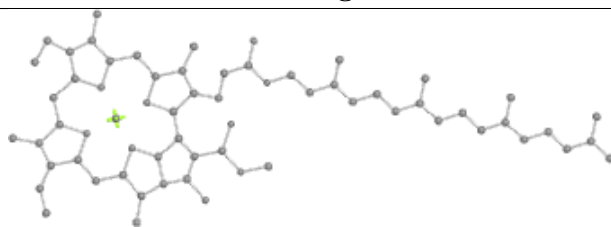
Bond lengths



Bond angles

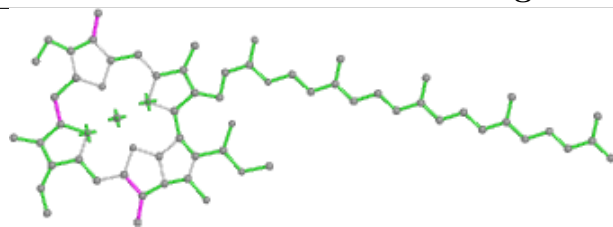


Torsions

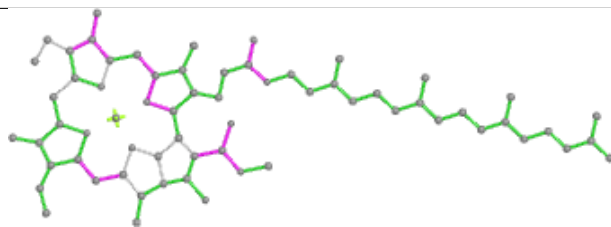


Rings

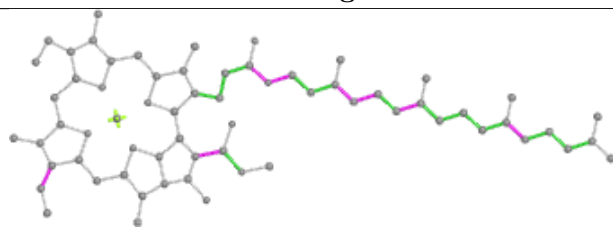
Ligand CLA B 807



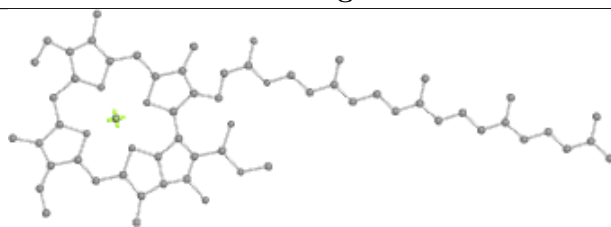
Bond lengths



Bond angles

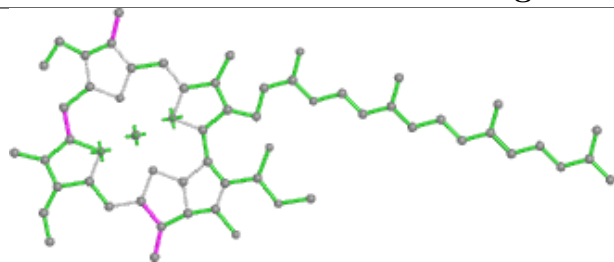


Torsions

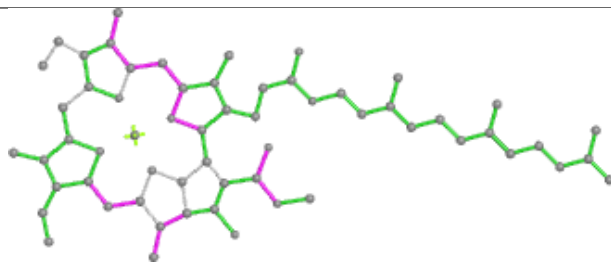


Rings

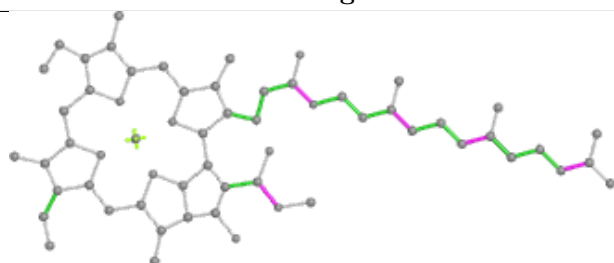
Ligand CLA B 808



Bond lengths



Bond angles

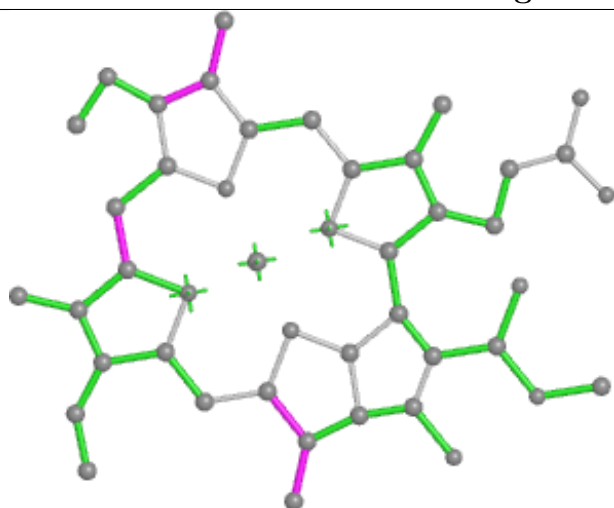


Torsions

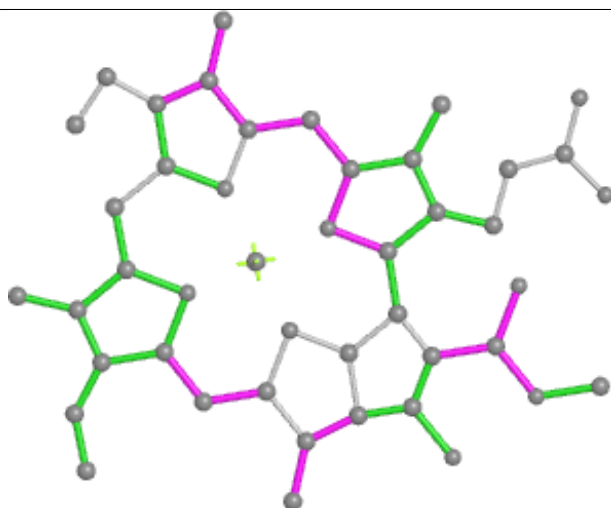


Rings

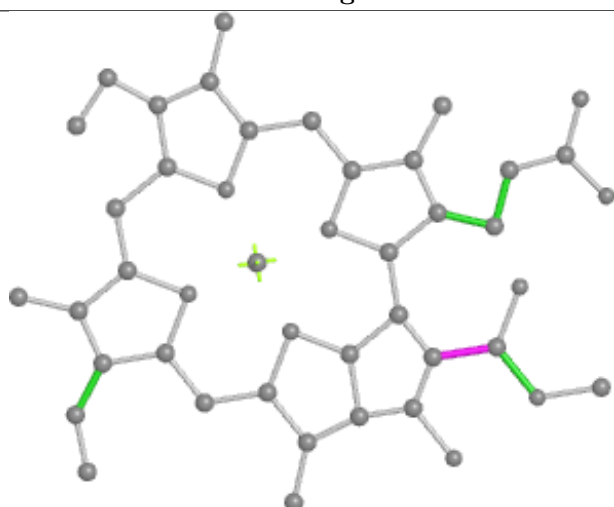
Ligand CLA B 809



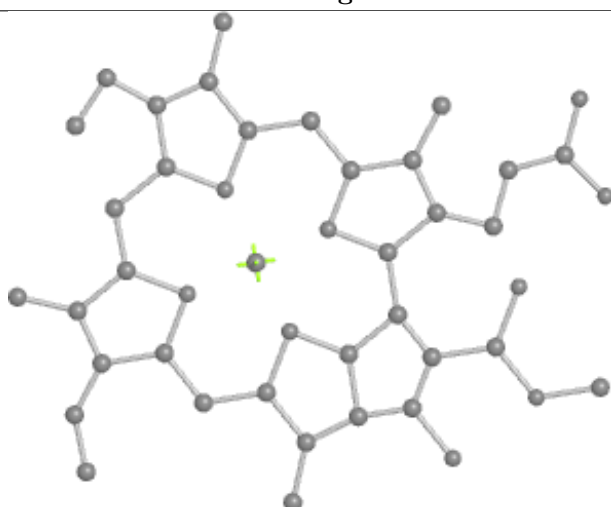
Bond lengths



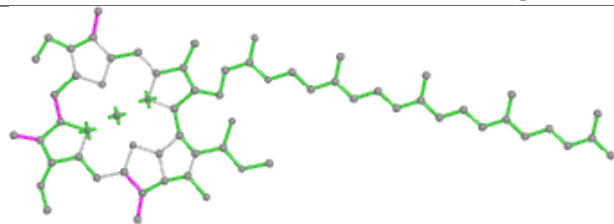
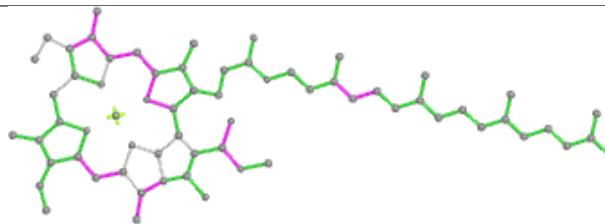
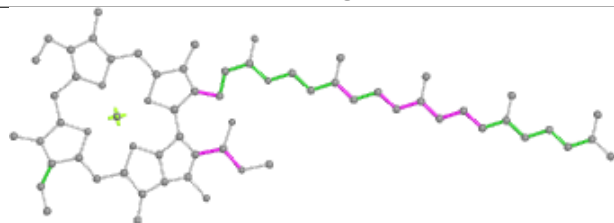
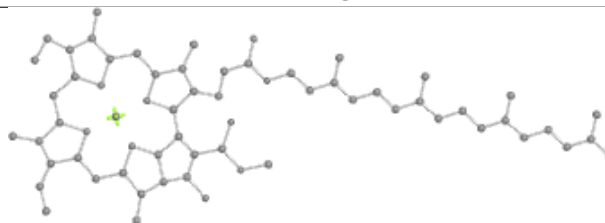
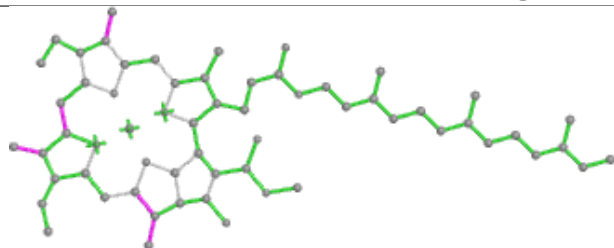
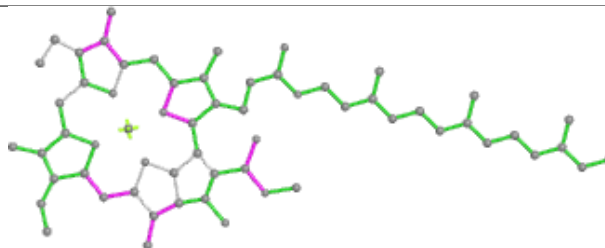
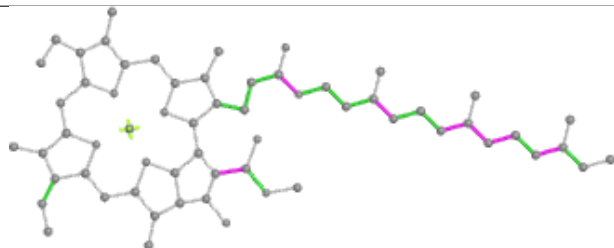
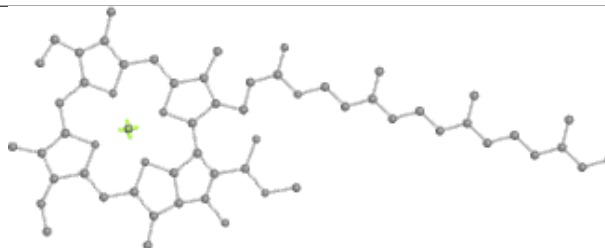
Bond angles



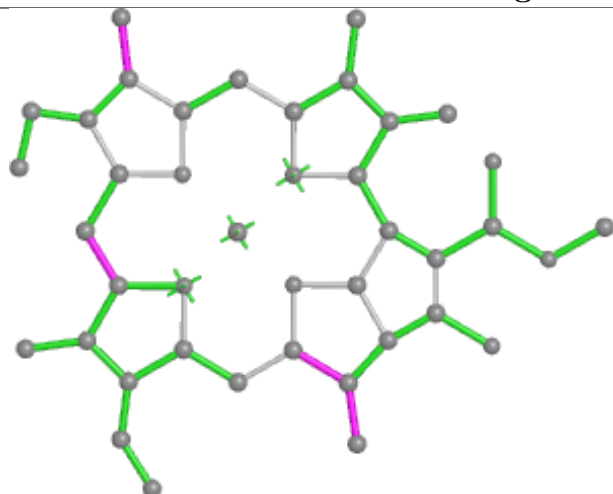
Torsions



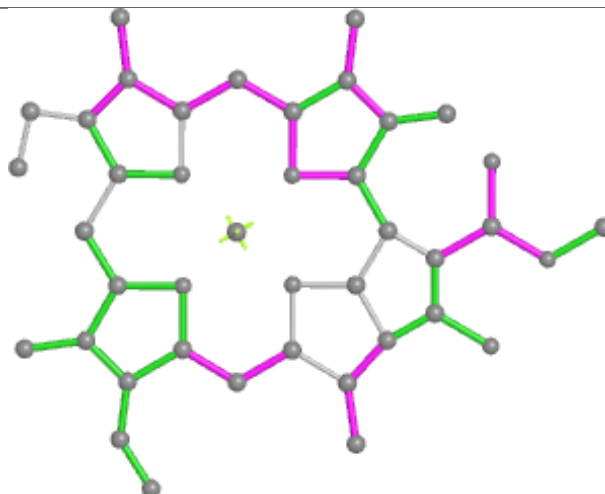
Rings

Ligand CLA B 810**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 811****Bond lengths****Bond angles****Torsions****Rings**

Ligand CLA B 812



Bond lengths



Bond angles

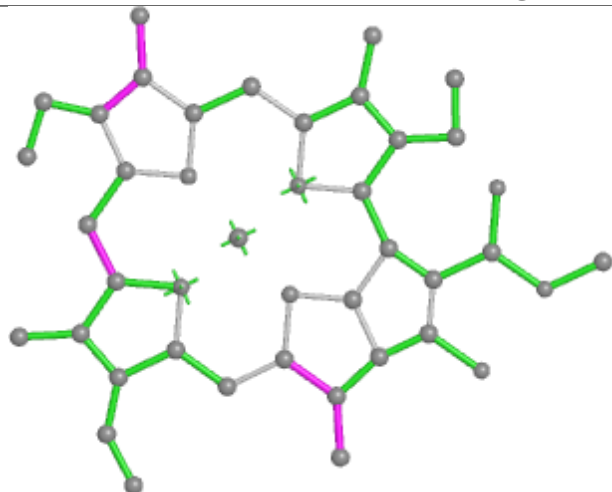


Torsions

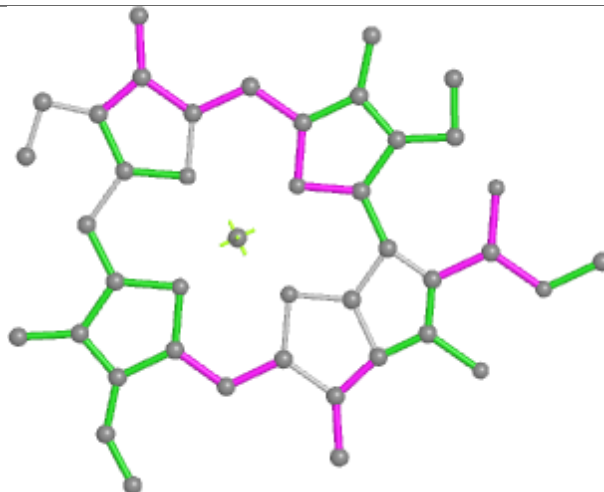


Rings

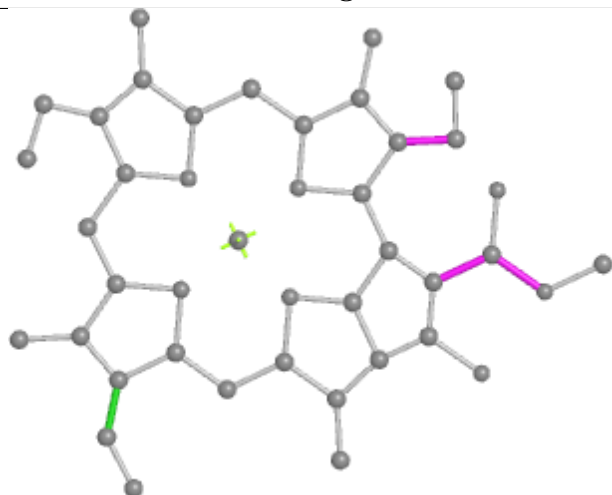
Ligand CLA B 813



Bond lengths



Bond angles

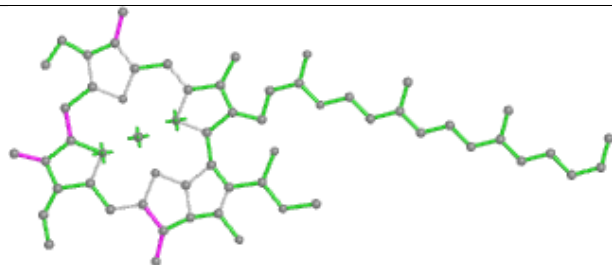


Torsions

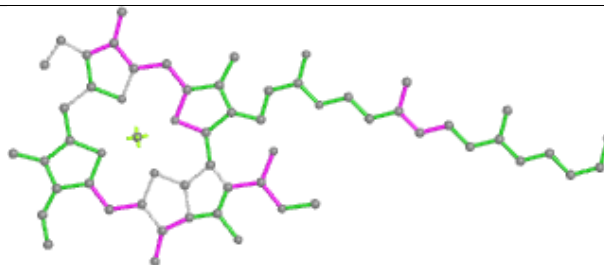


Rings

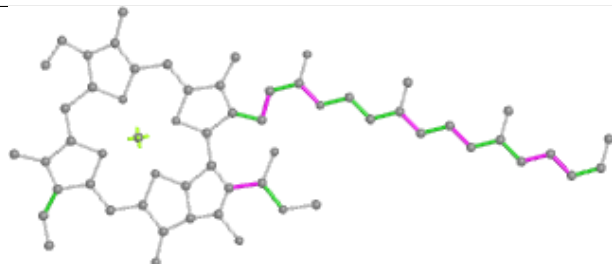
Ligand CLA B 814



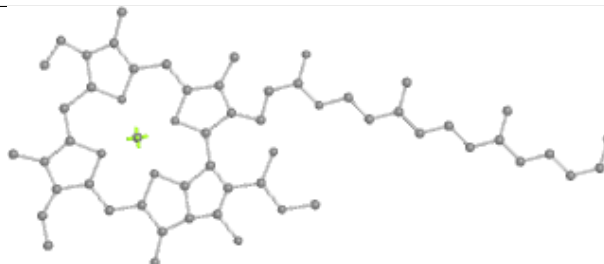
Bond lengths



Bond angles

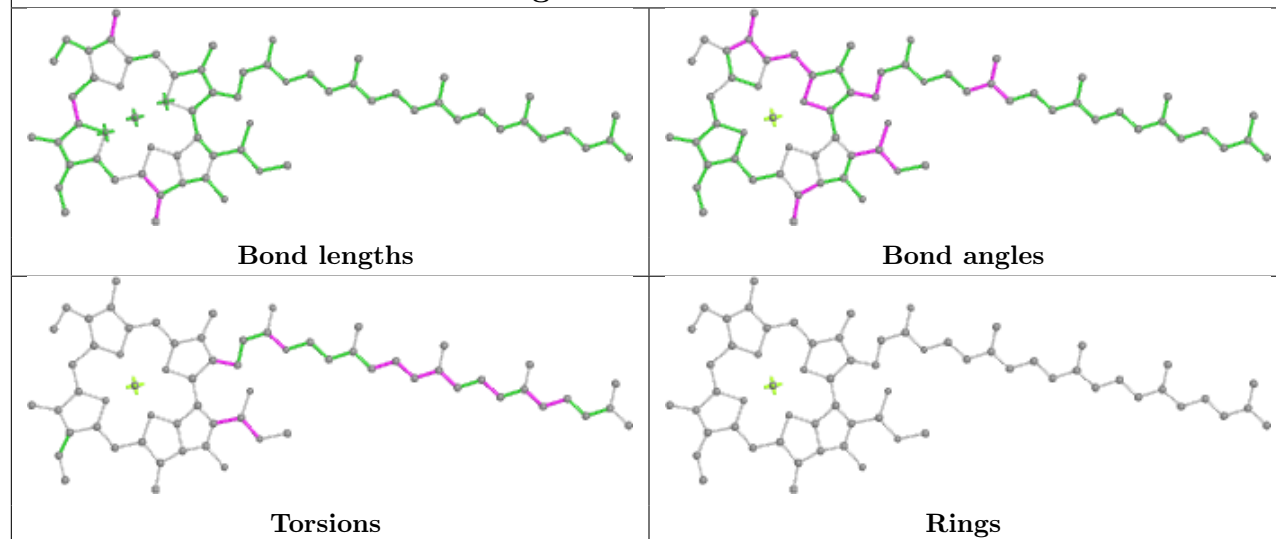


Torsions

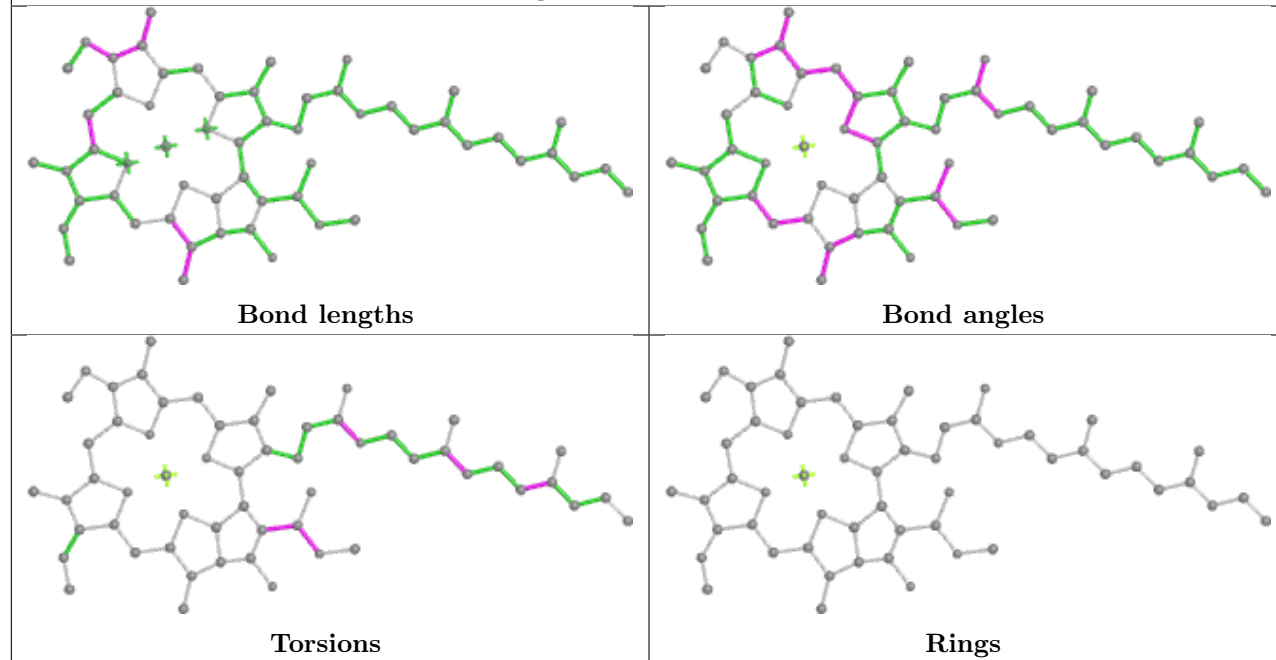


Rings

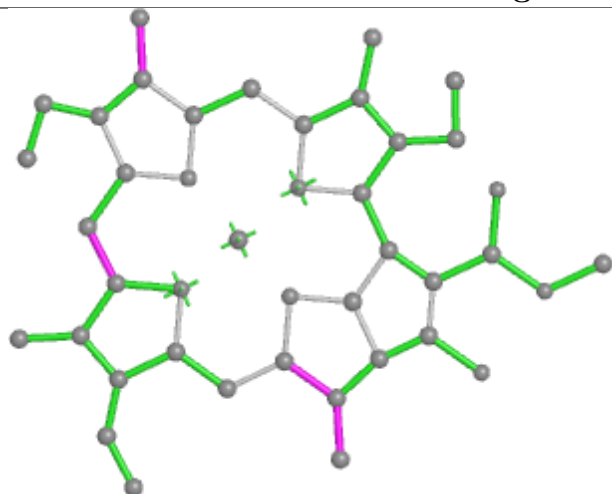
Ligand CLA B 815



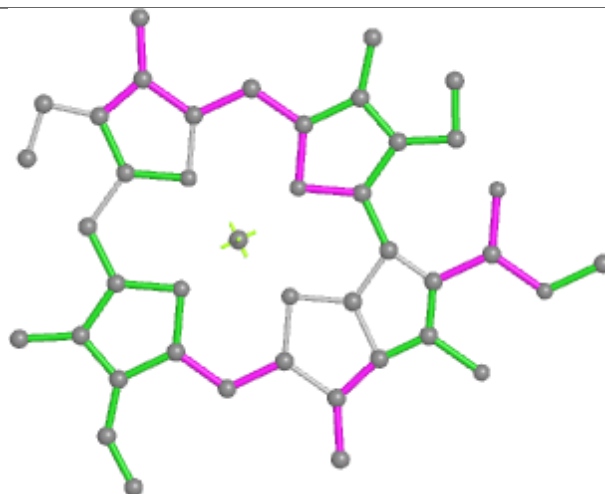
Ligand CLA B 816



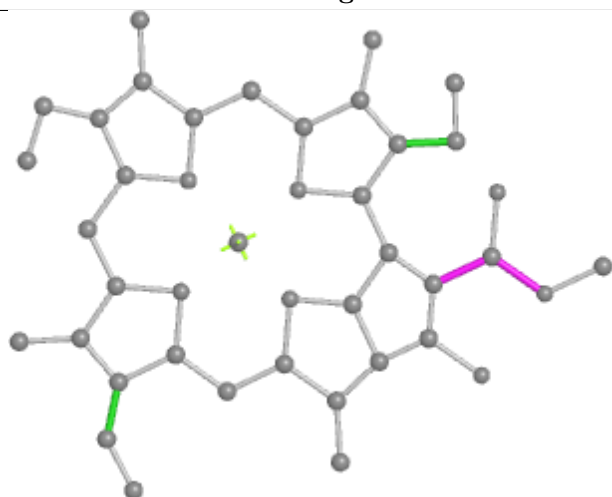
Ligand CLA B 817



Bond lengths



Bond angles

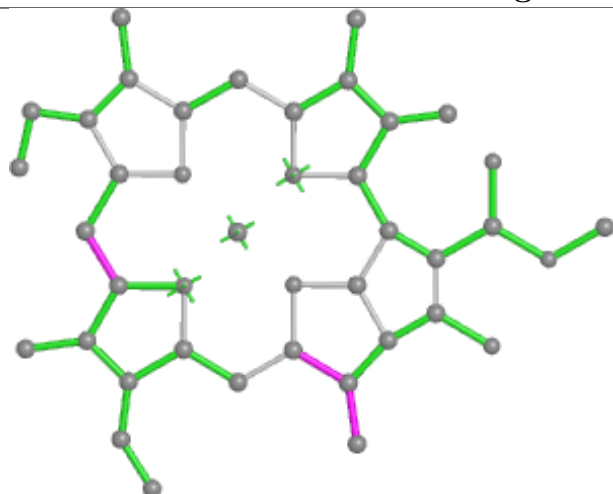


Torsions

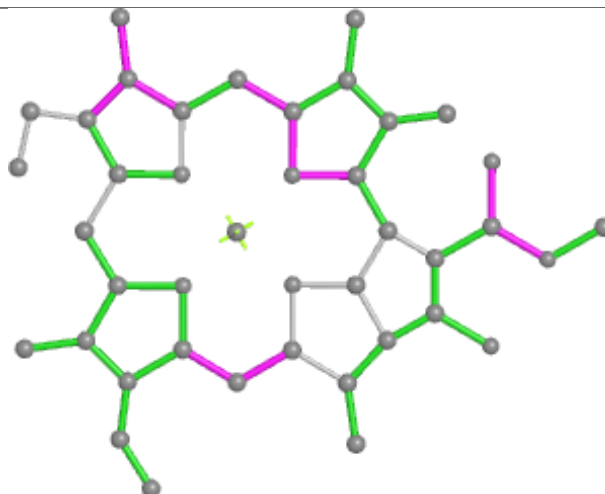


Rings

Ligand CLA B 818



Bond lengths



Bond angles

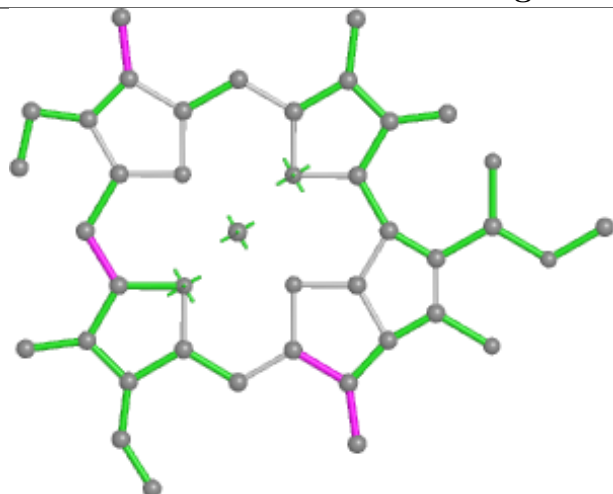


Torsions

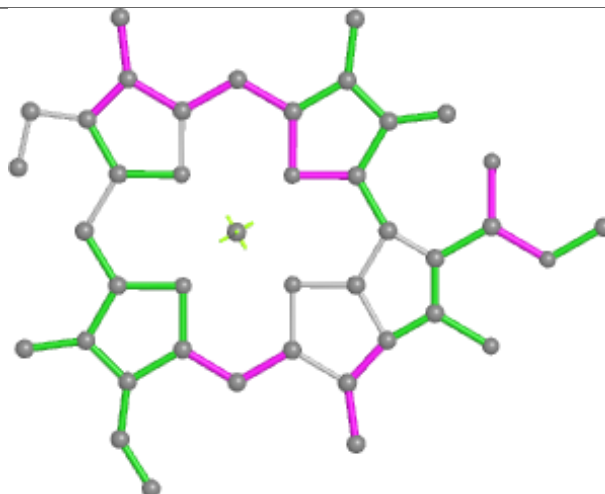


Rings

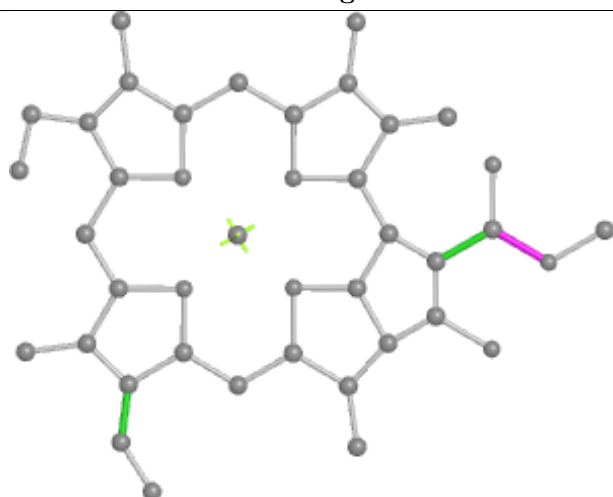
Ligand CLA B 819



Bond lengths



Bond angles

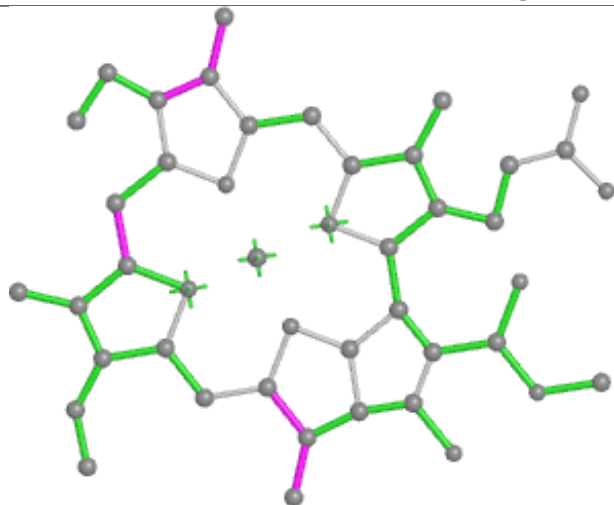


Torsions

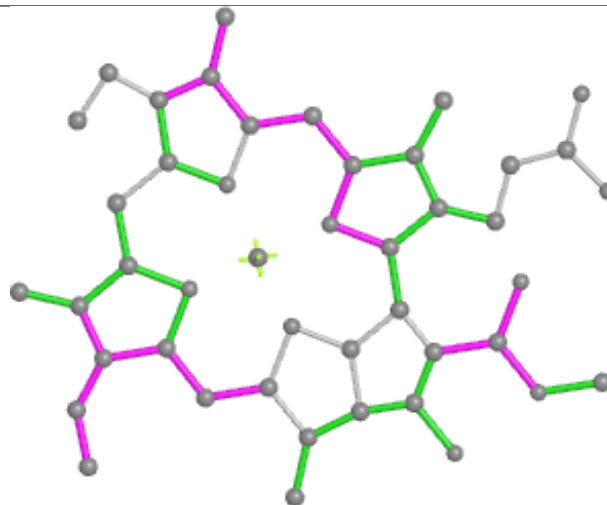


Rings

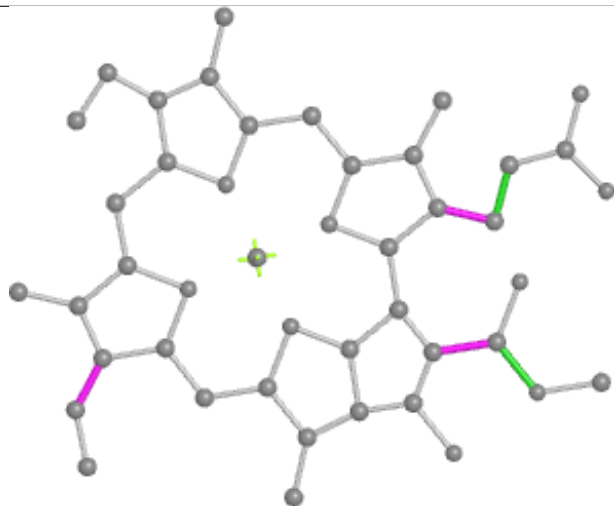
Ligand CLA B 820



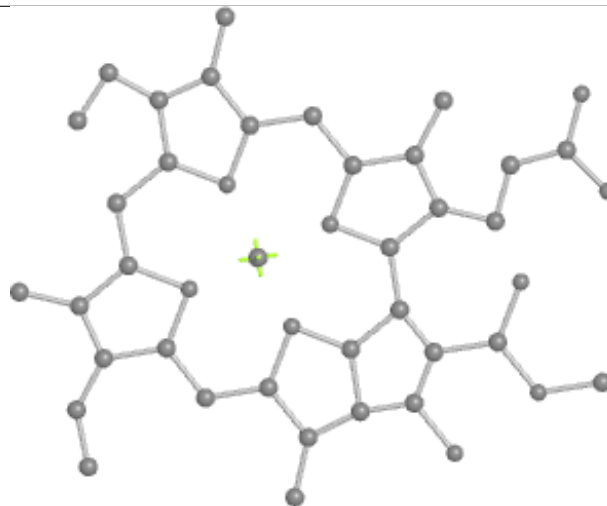
Bond lengths



Bond angles

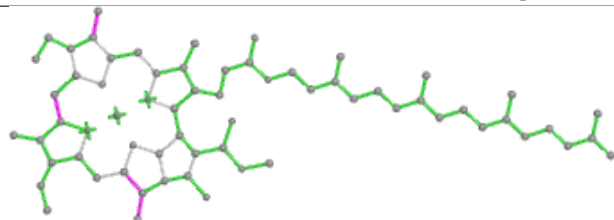


Torsions

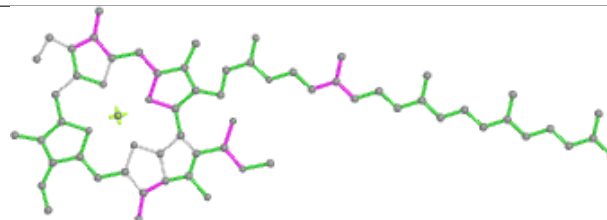


Rings

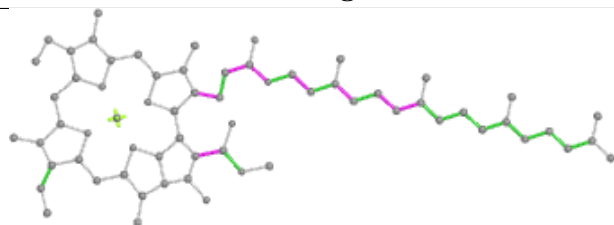
Ligand CLA B 821



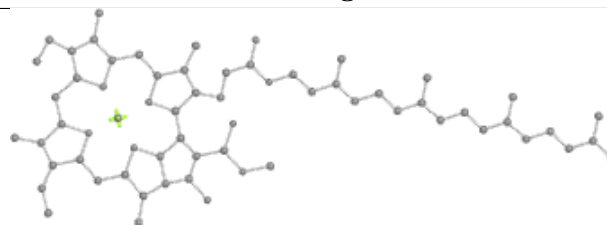
Bond lengths



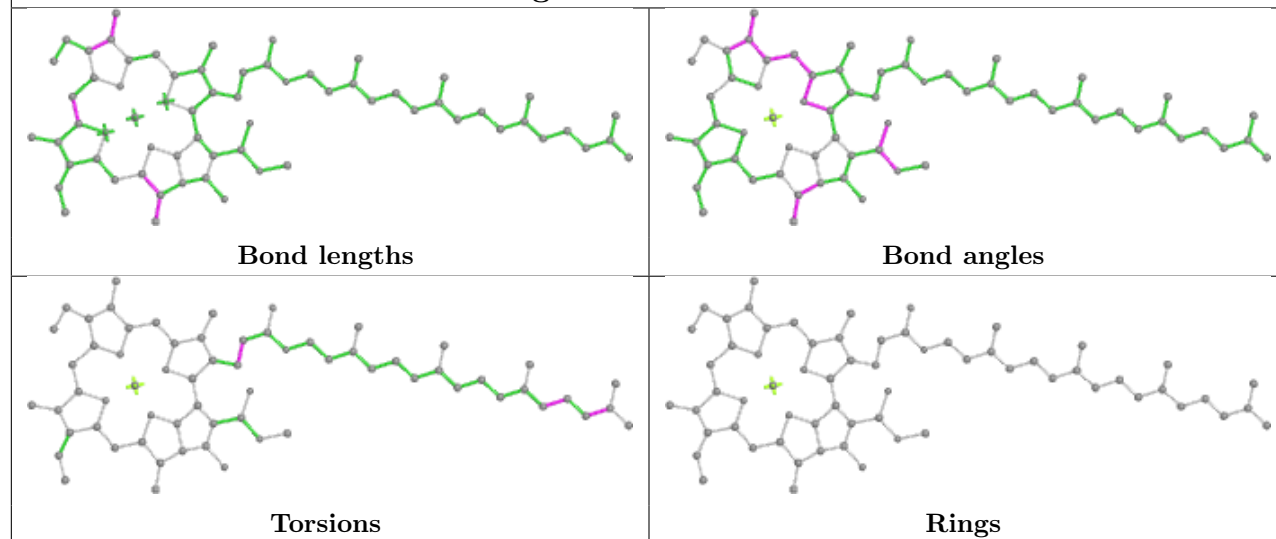
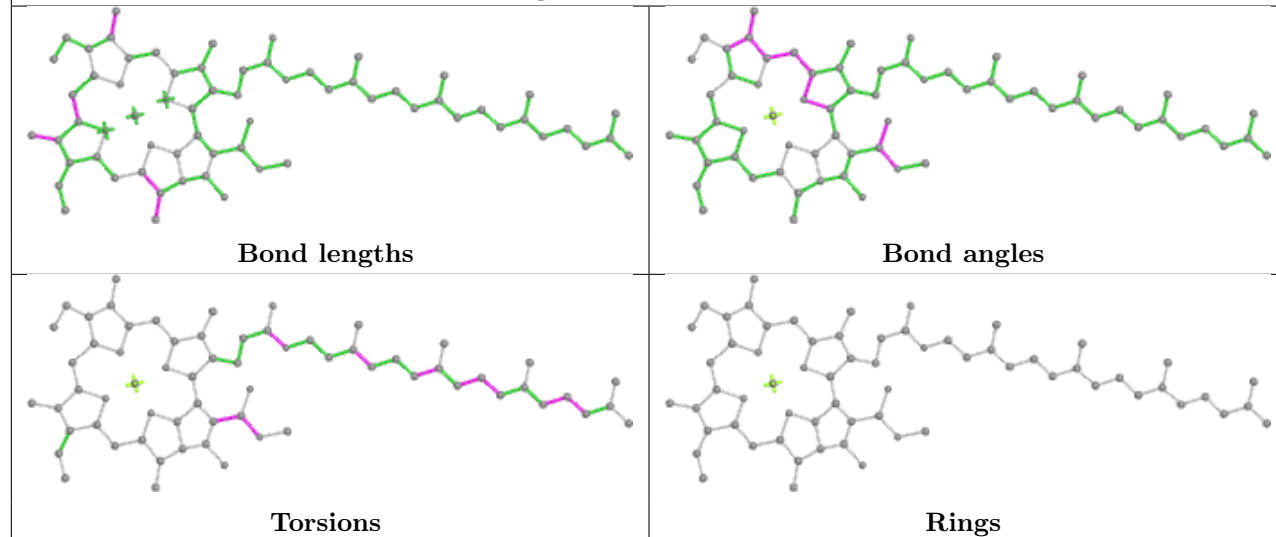
Bond angles

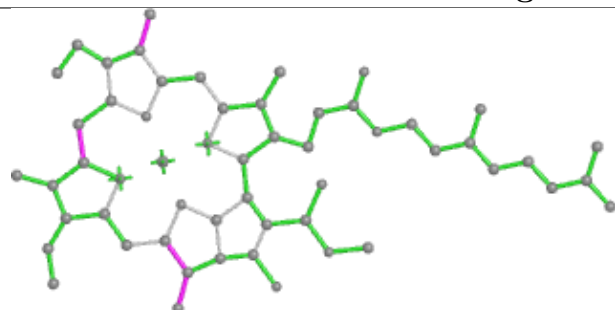


Torsions

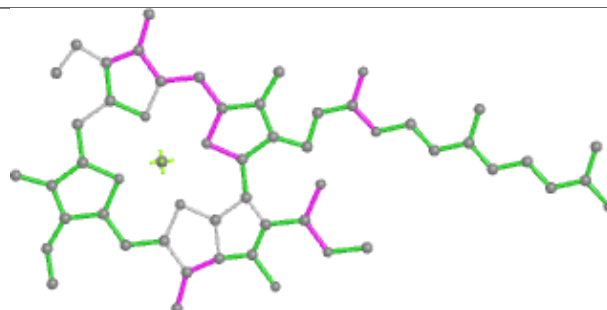


Rings

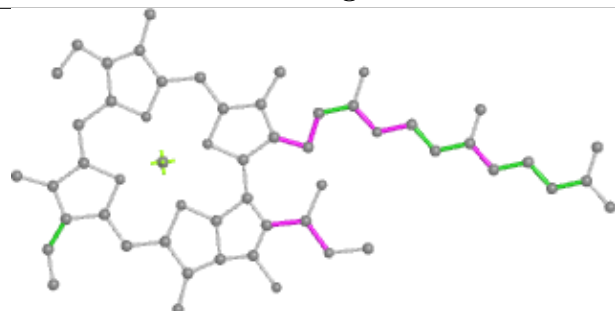
Ligand CLA B 822**Ligand CLA B 823**

Ligand CLA B 824

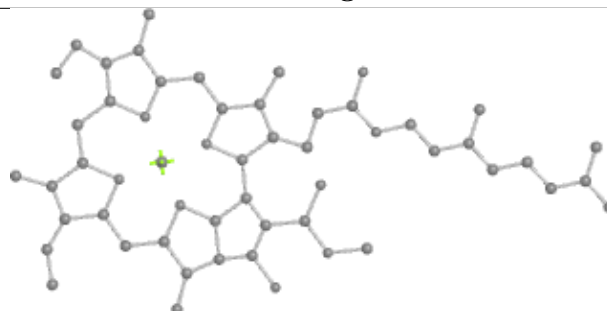
Bond lengths



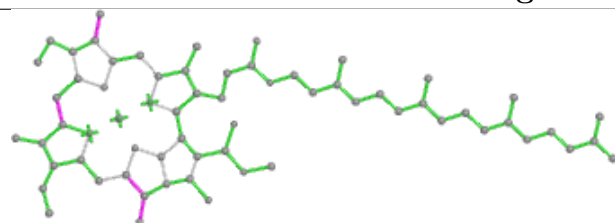
Bond angles



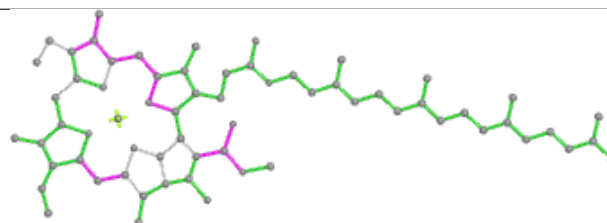
Torsions



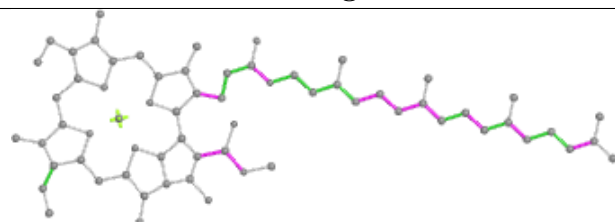
Rings

Ligand CLA B 825

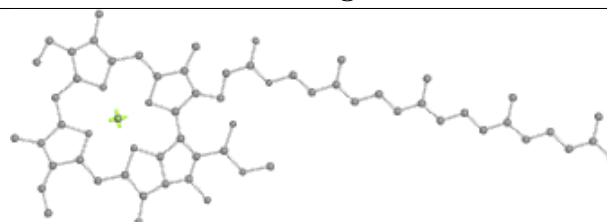
Bond lengths



Bond angles

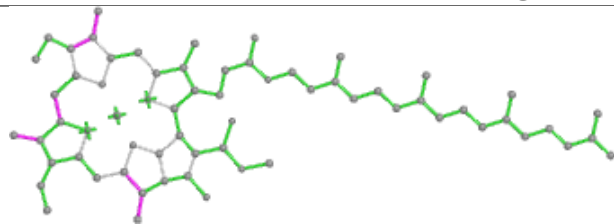


Torsions

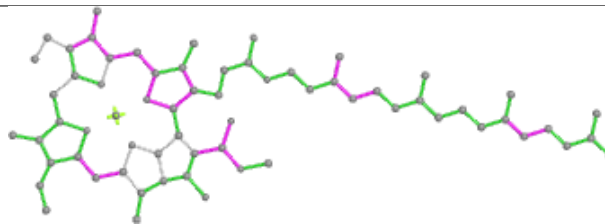


Rings

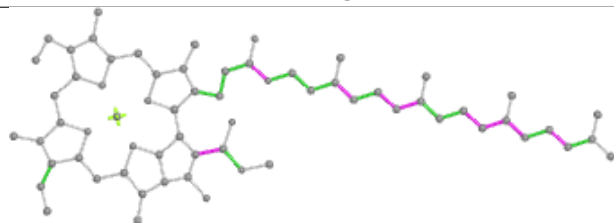
Ligand CLA B 826



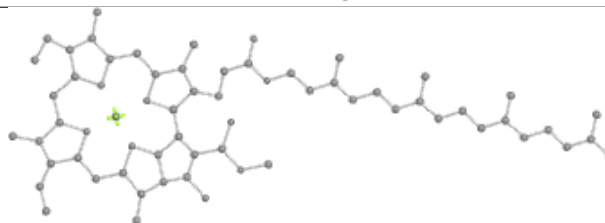
Bond lengths



Bond angles

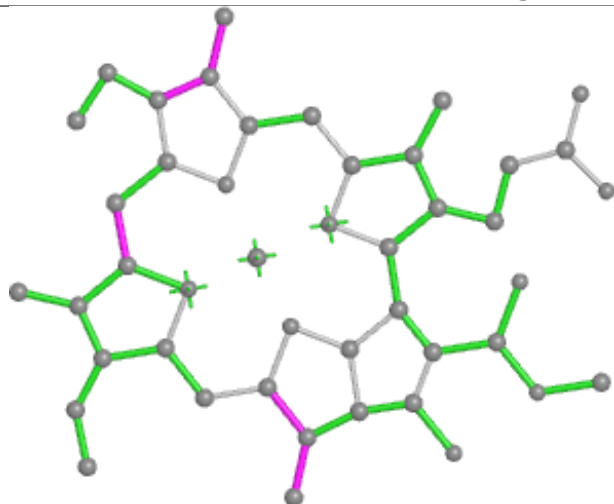


Torsions

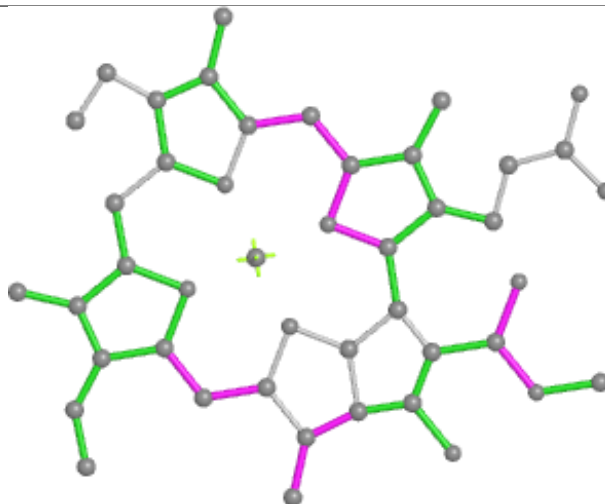


Rings

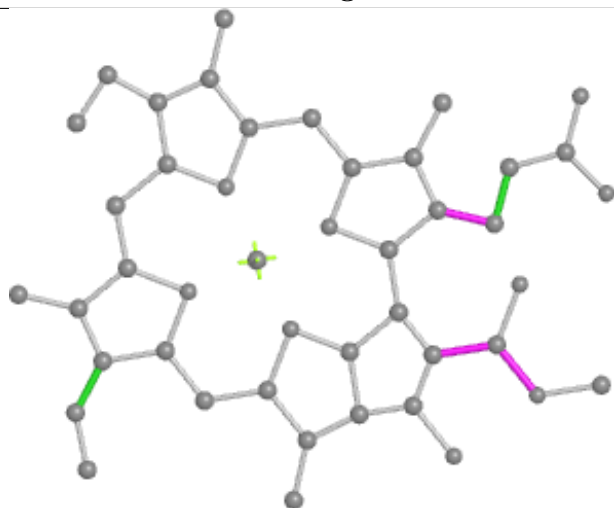
Ligand CLA B 827



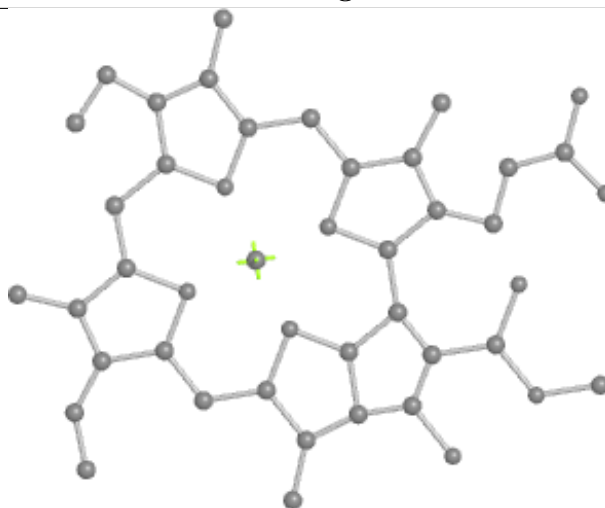
Bond lengths



Bond angles

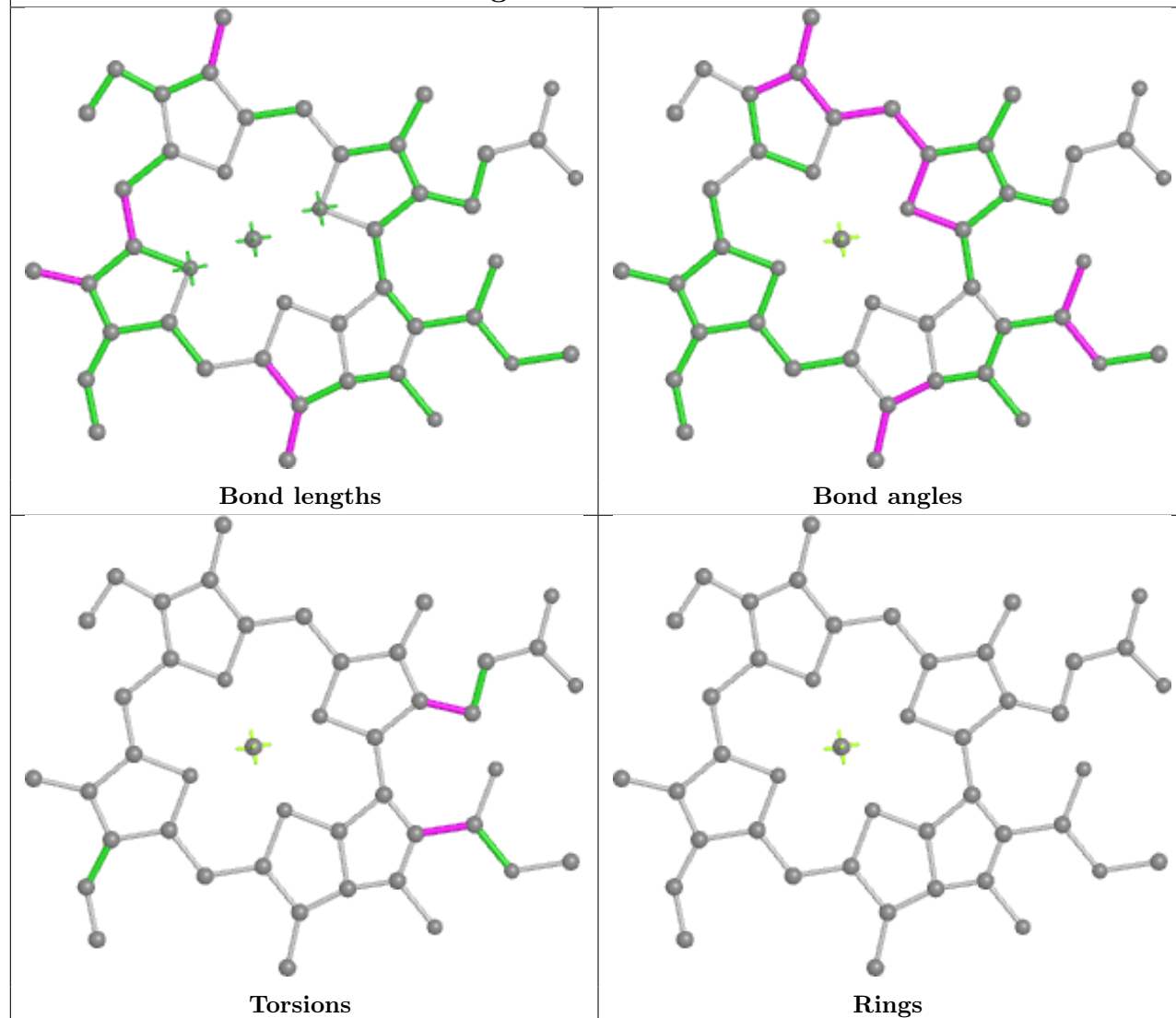


Torsions

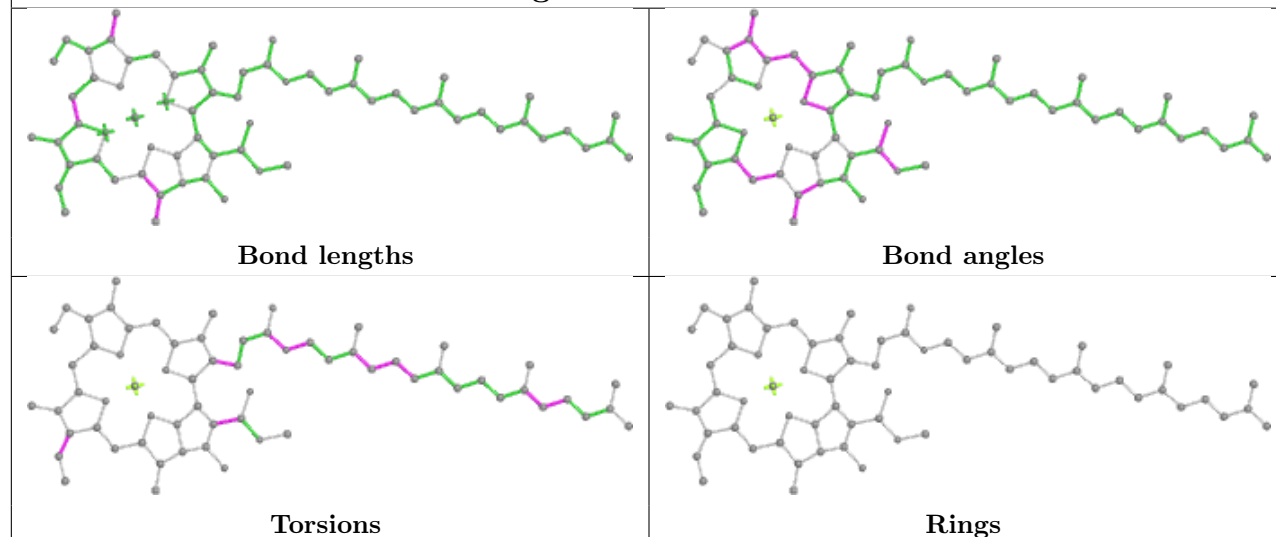


Rings

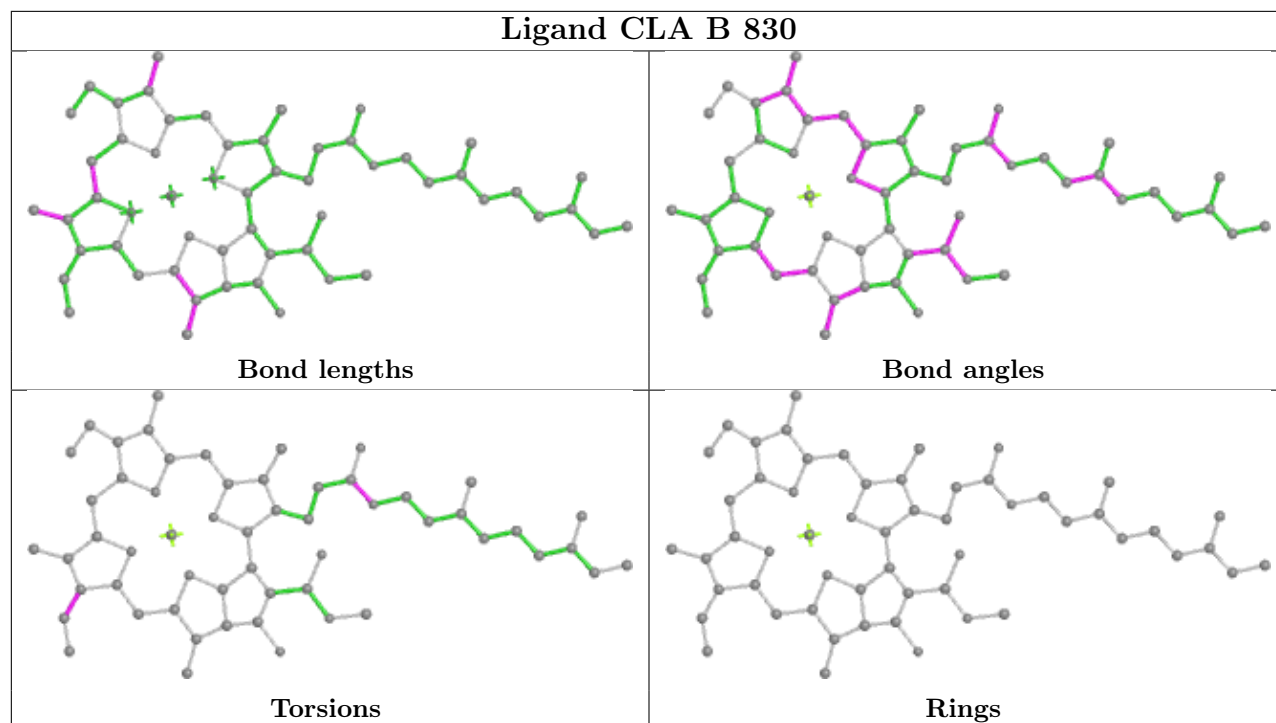
Ligand CLA B 828



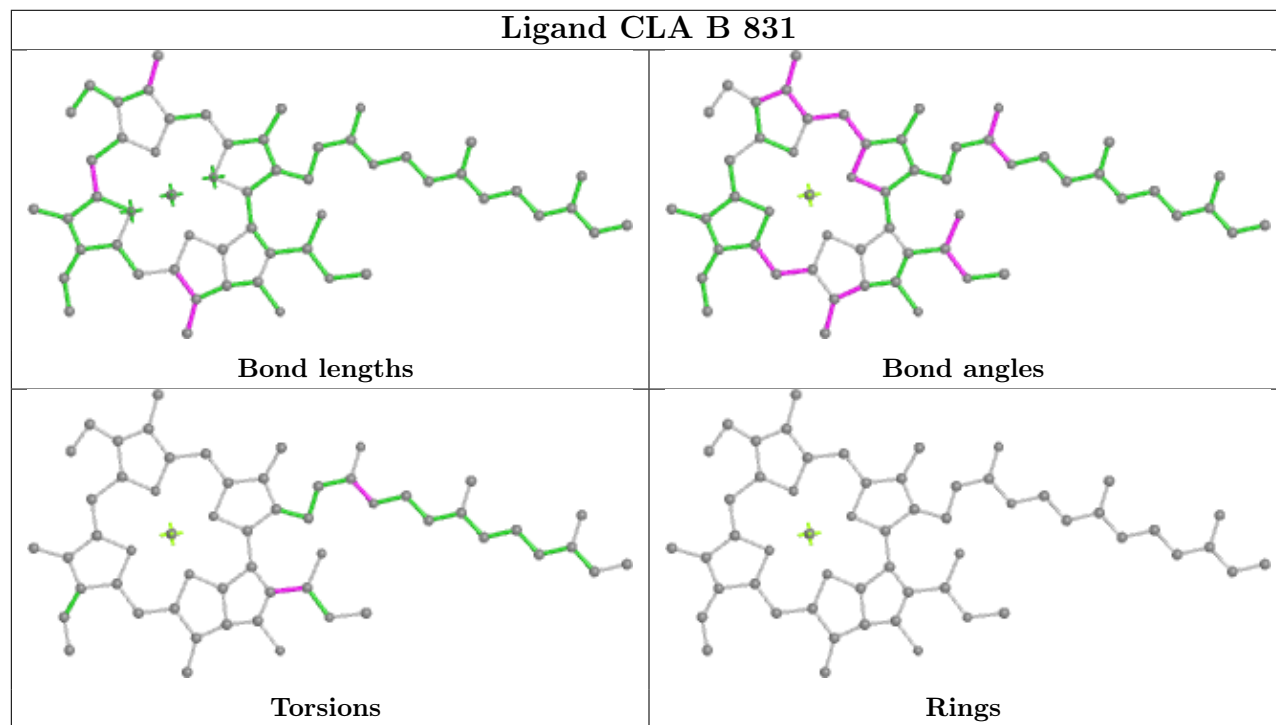
Ligand CLA B 829



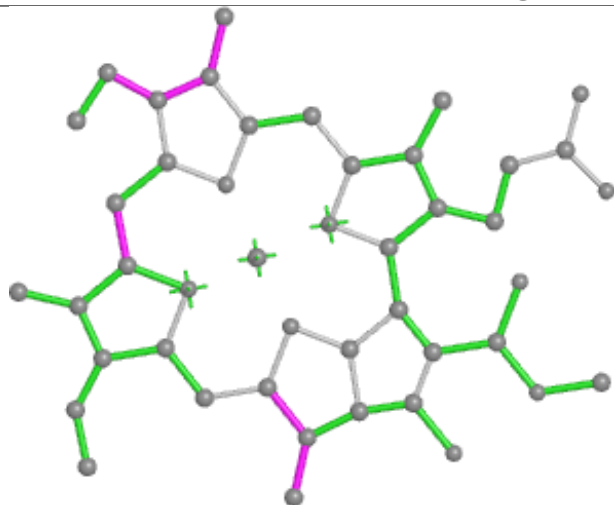
Ligand CLA B 830



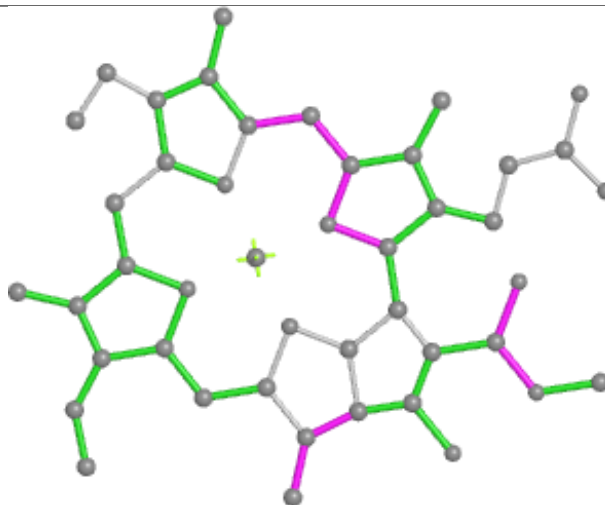
Ligand CLA B 831



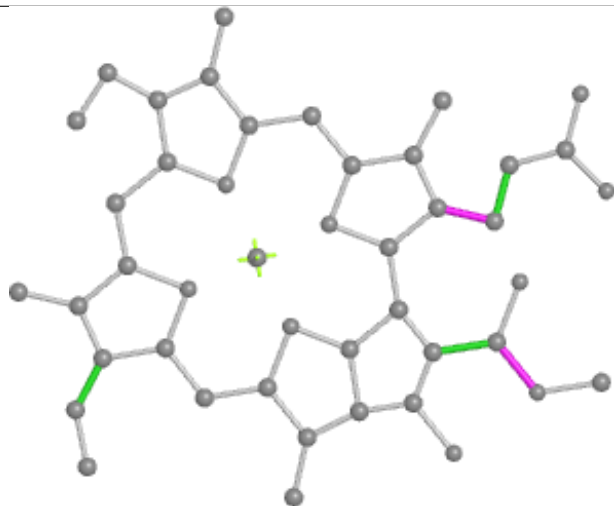
Ligand CLA B 832



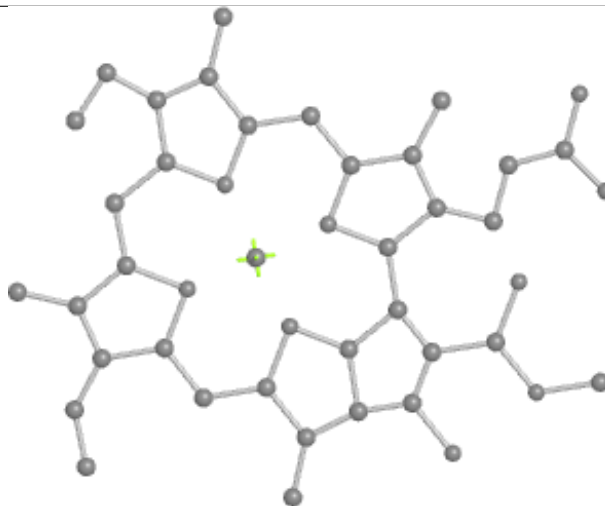
Bond lengths



Bond angles

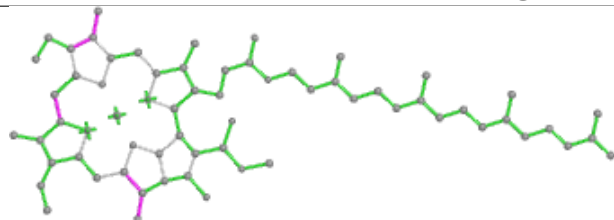


Torsions

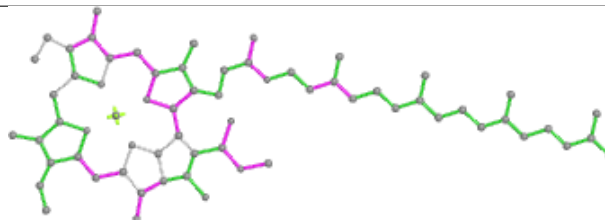


Rings

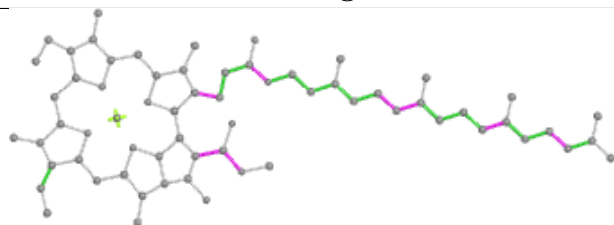
Ligand CLA B 833



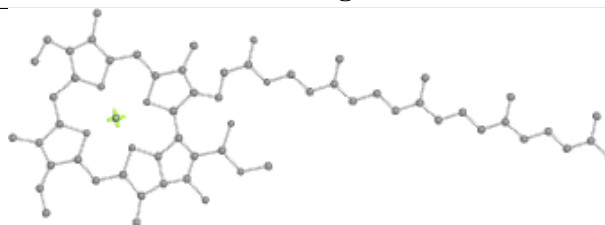
Bond lengths



Bond angles

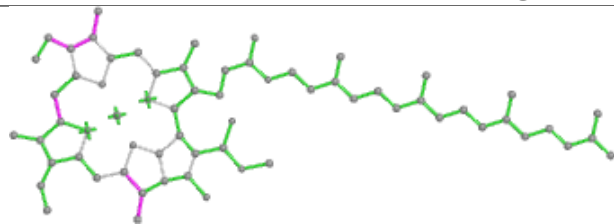


Torsions

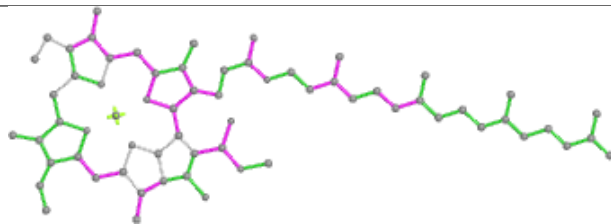


Rings

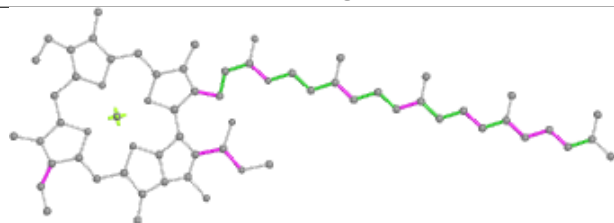
Ligand CLA B 834



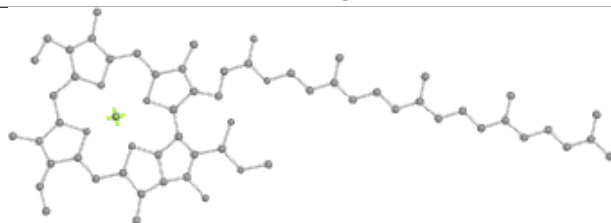
Bond lengths



Bond angles

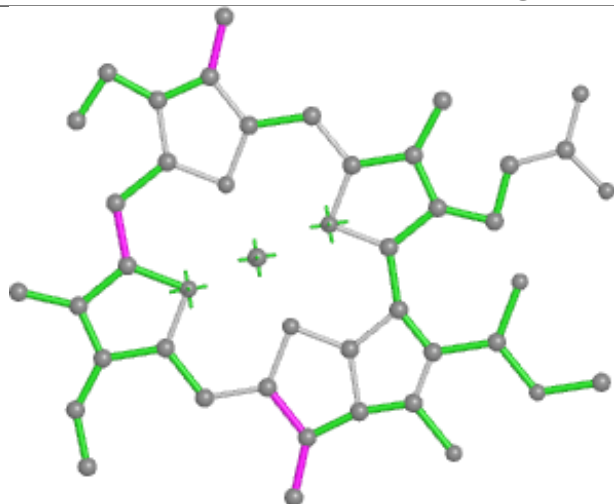


Torsions

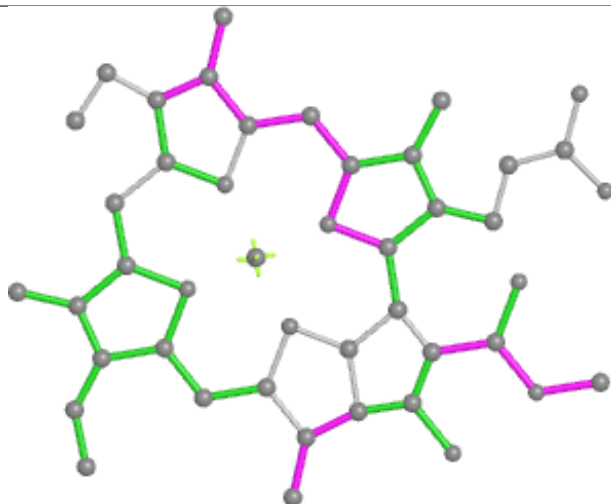


Rings

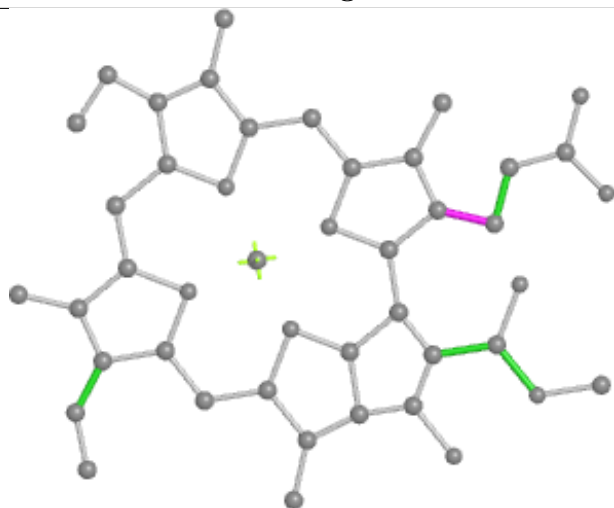
Ligand CLA B 835



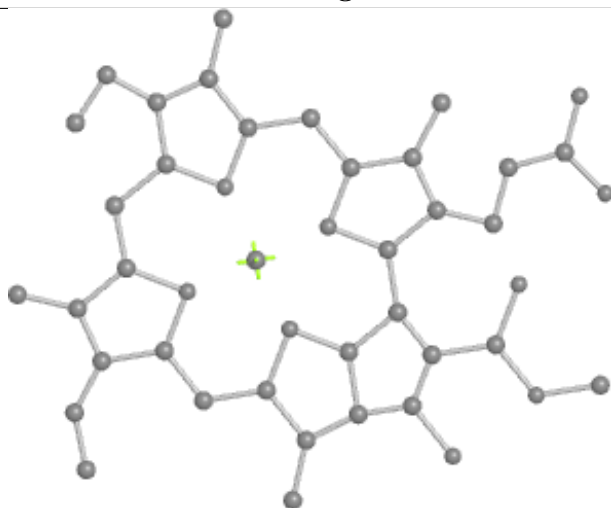
Bond lengths



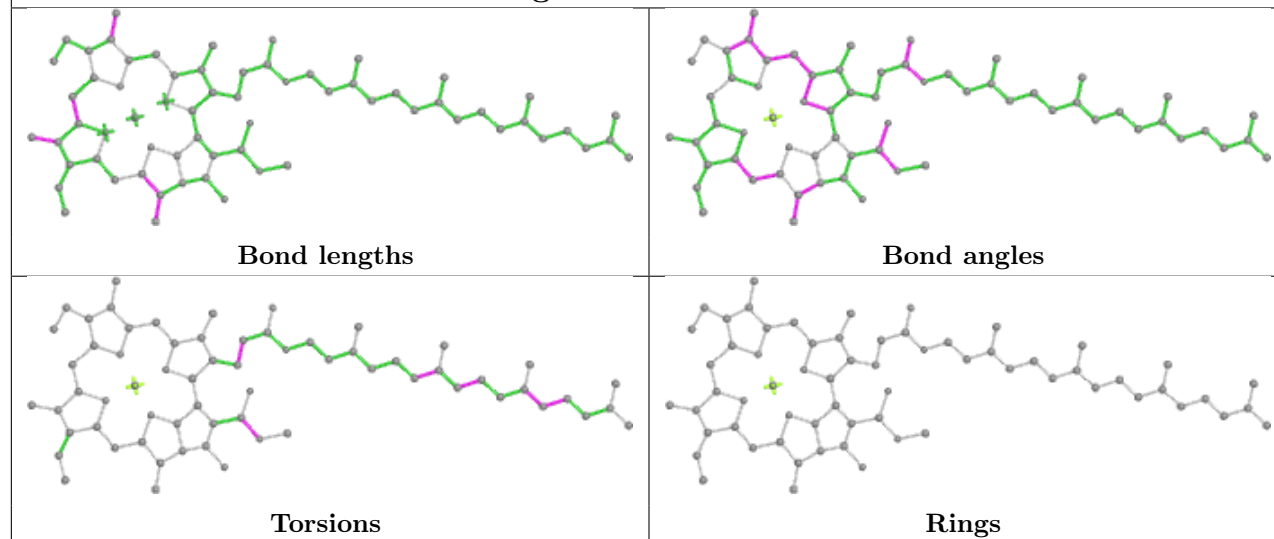
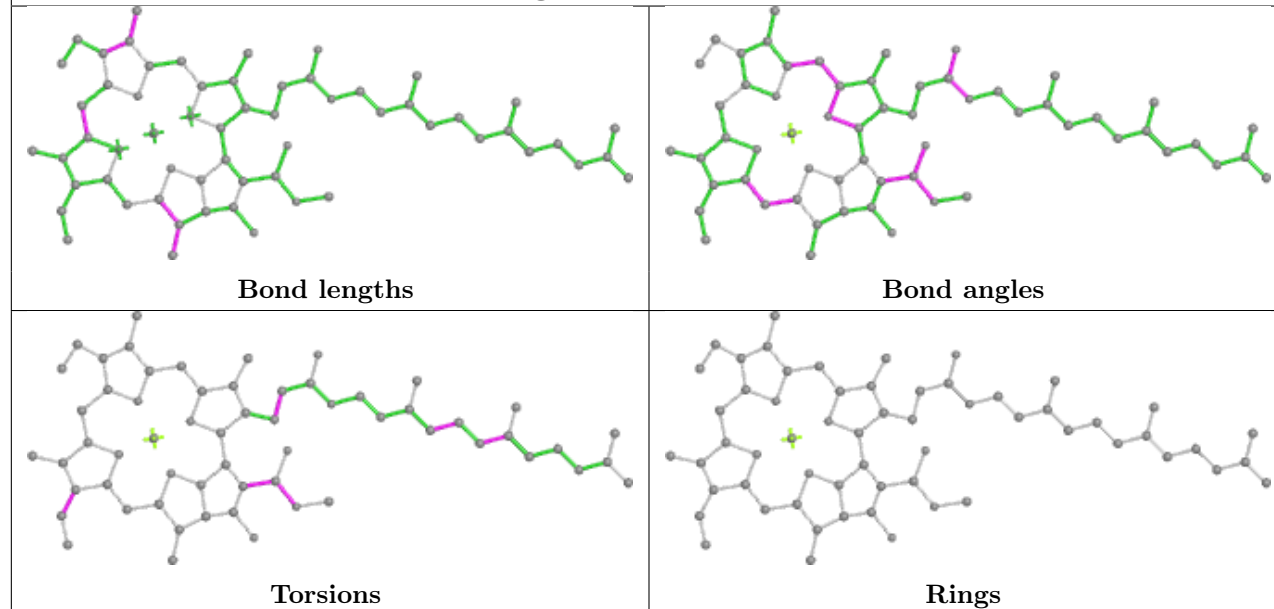
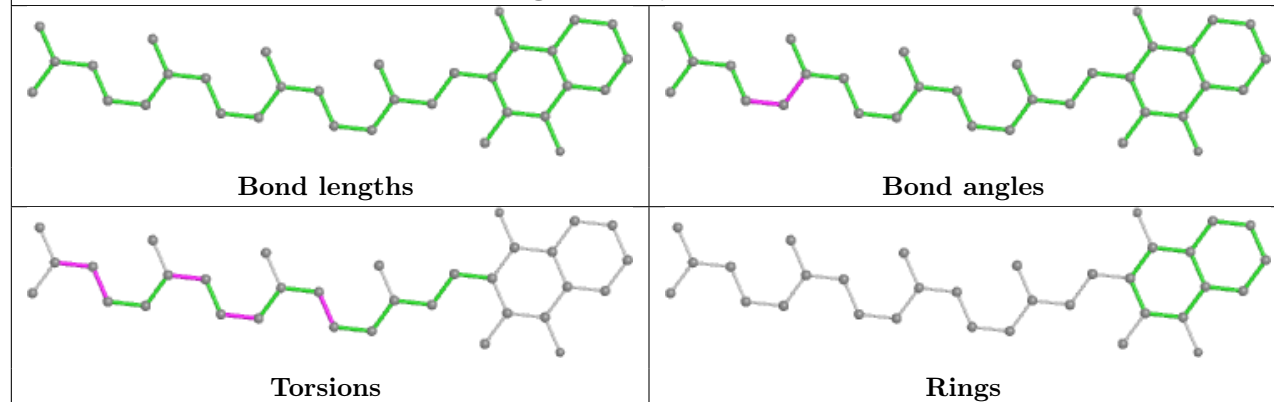
Bond angles

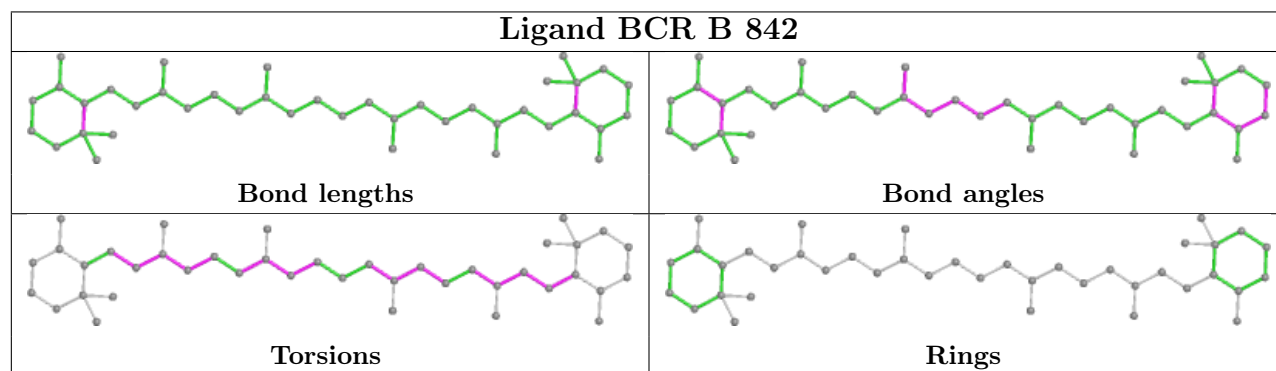
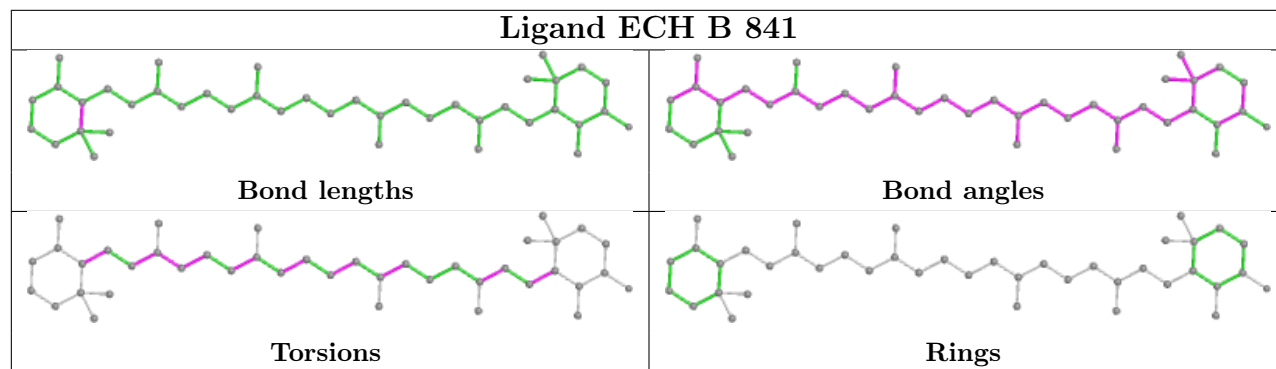
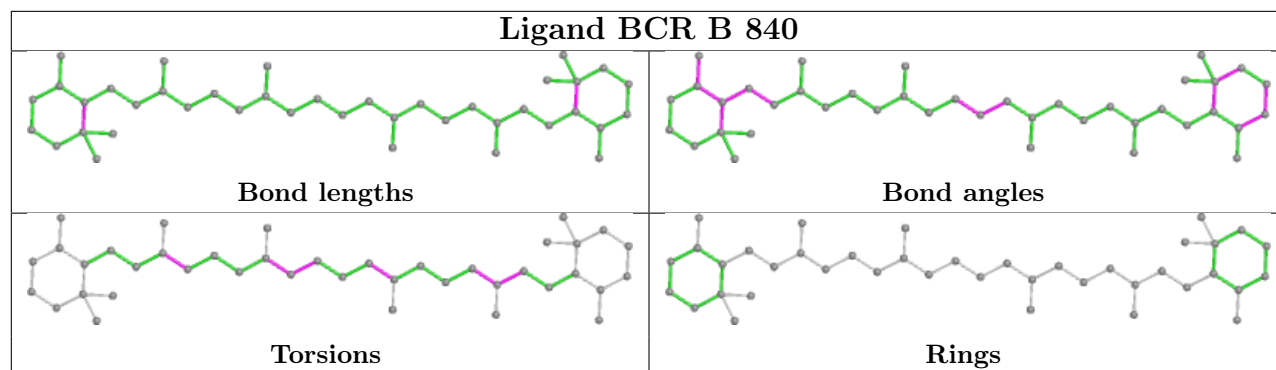
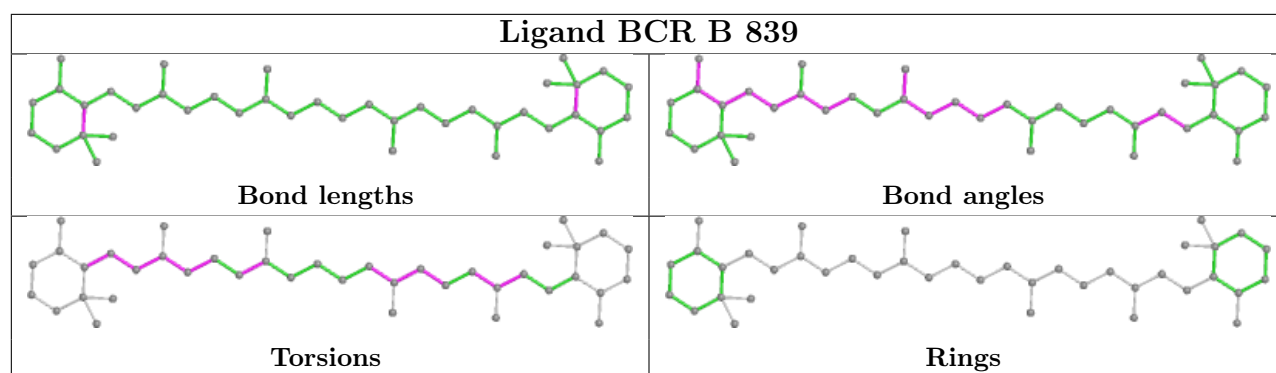


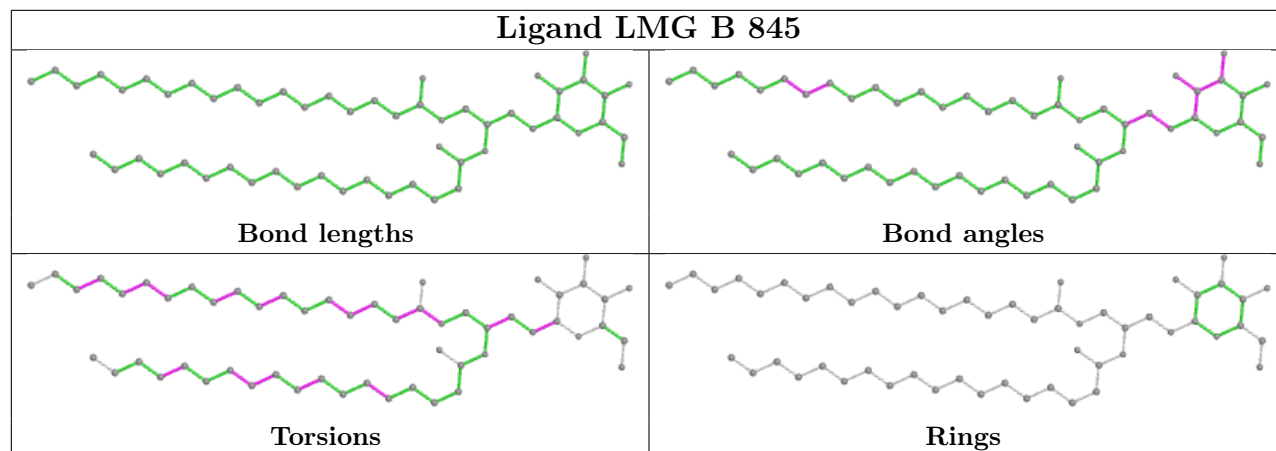
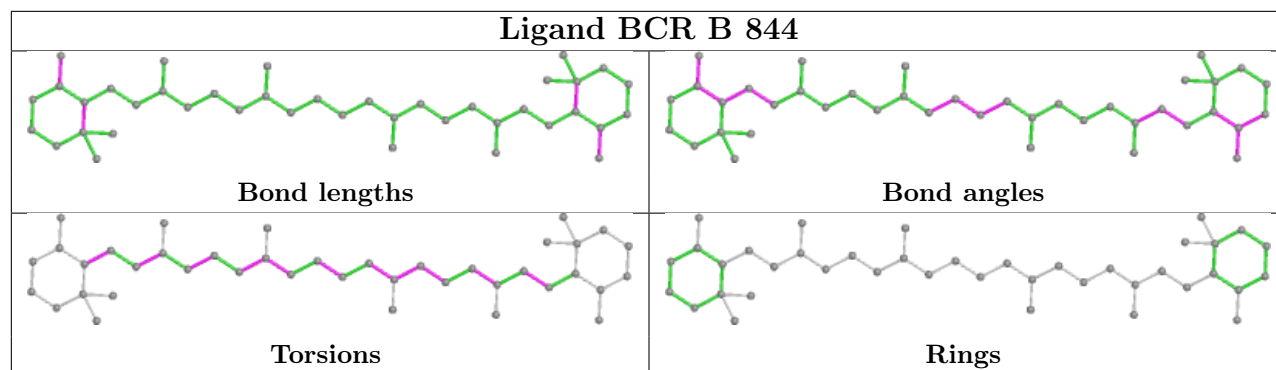
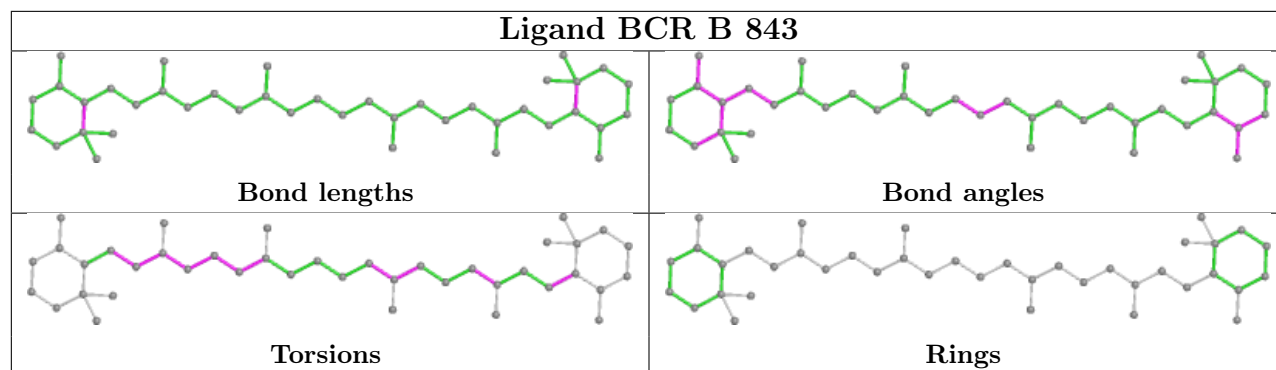
Torsions



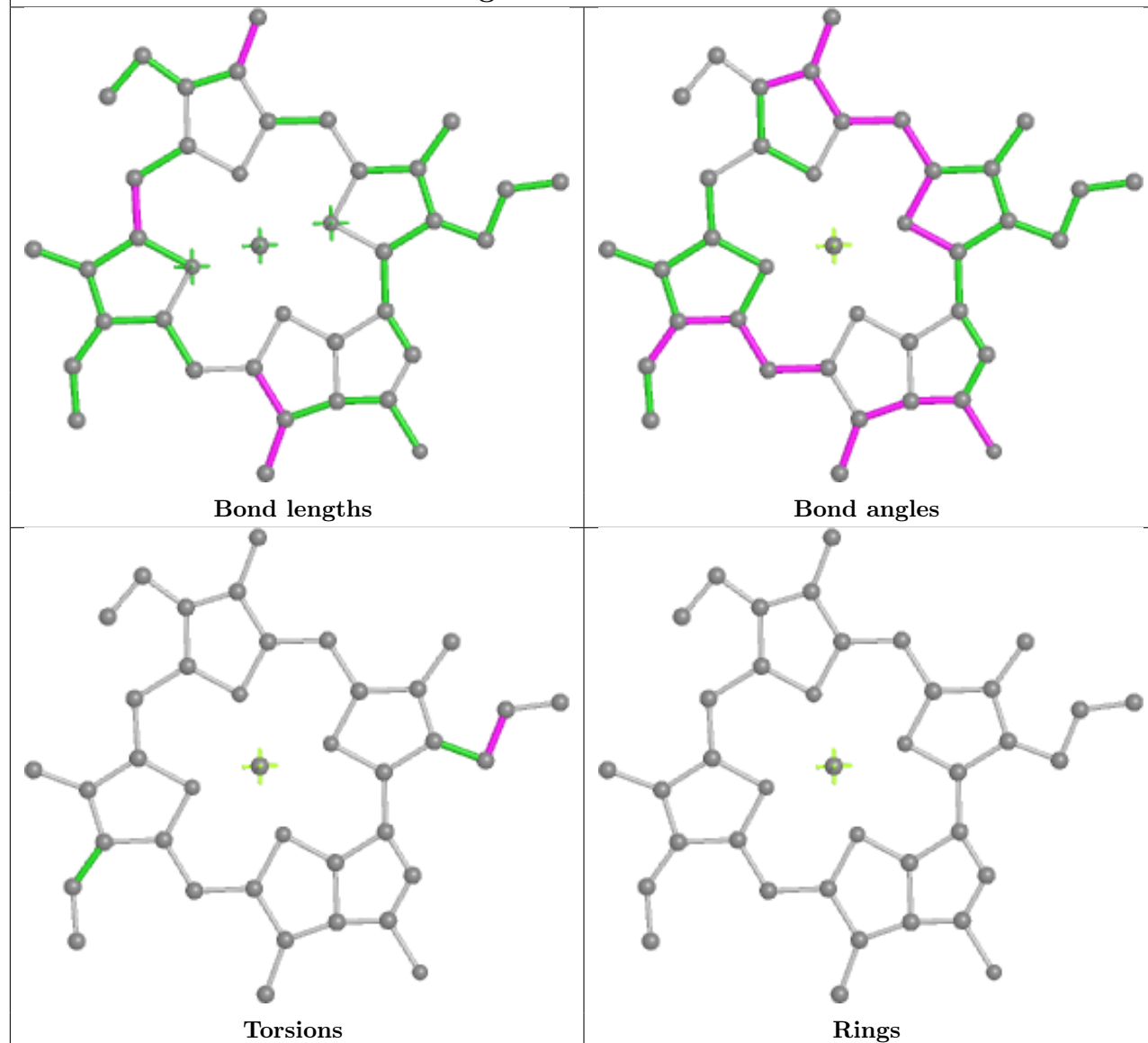
Rings

Ligand CLA B 836**Ligand CLA B 837****Ligand PQN B 838**

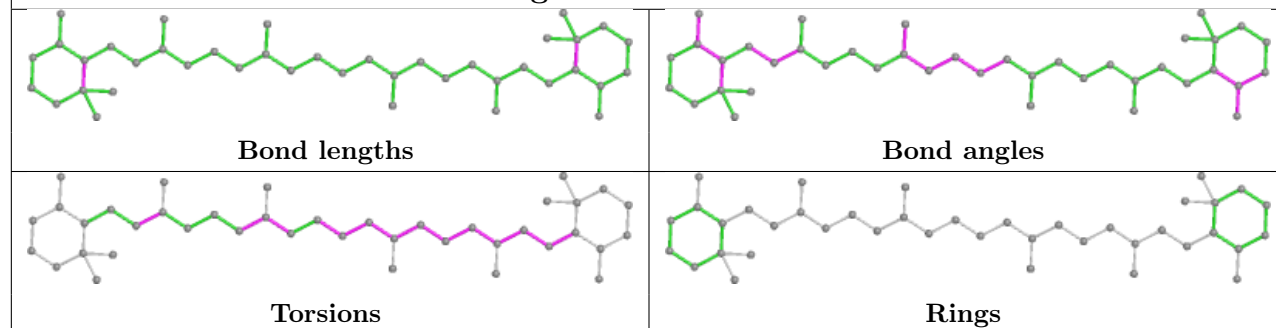


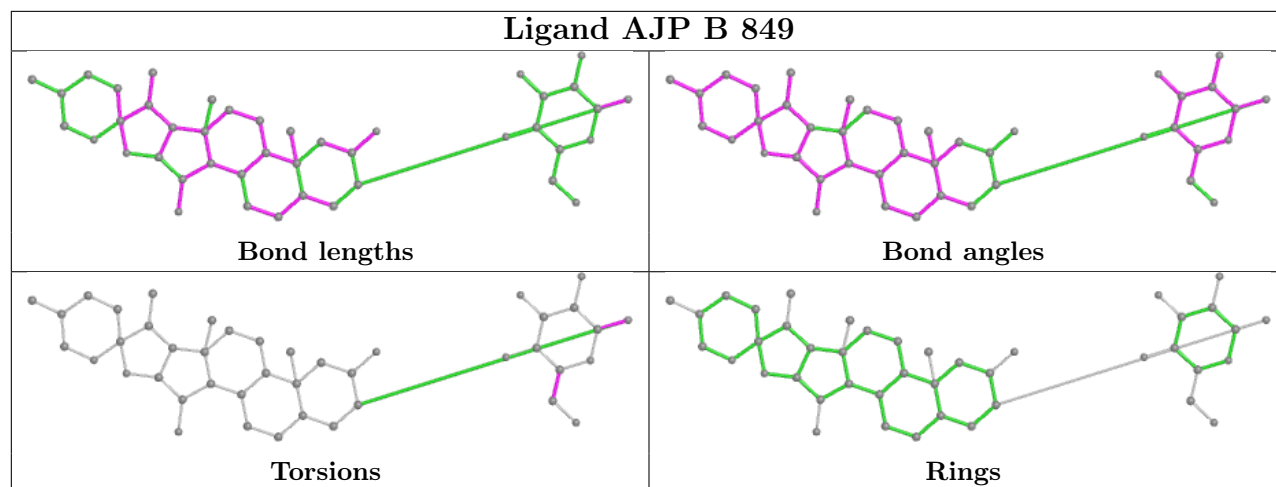
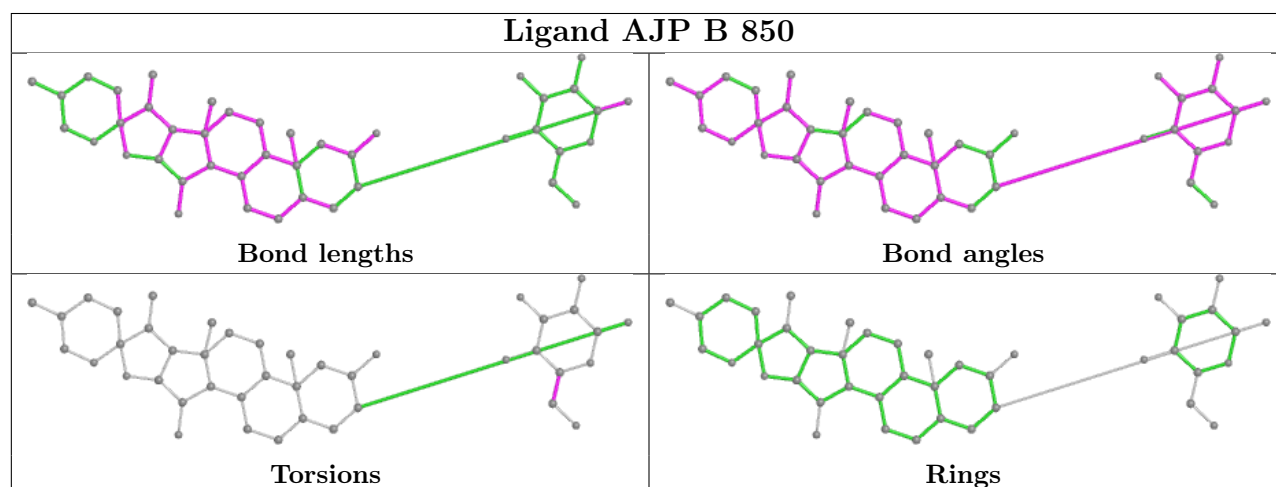
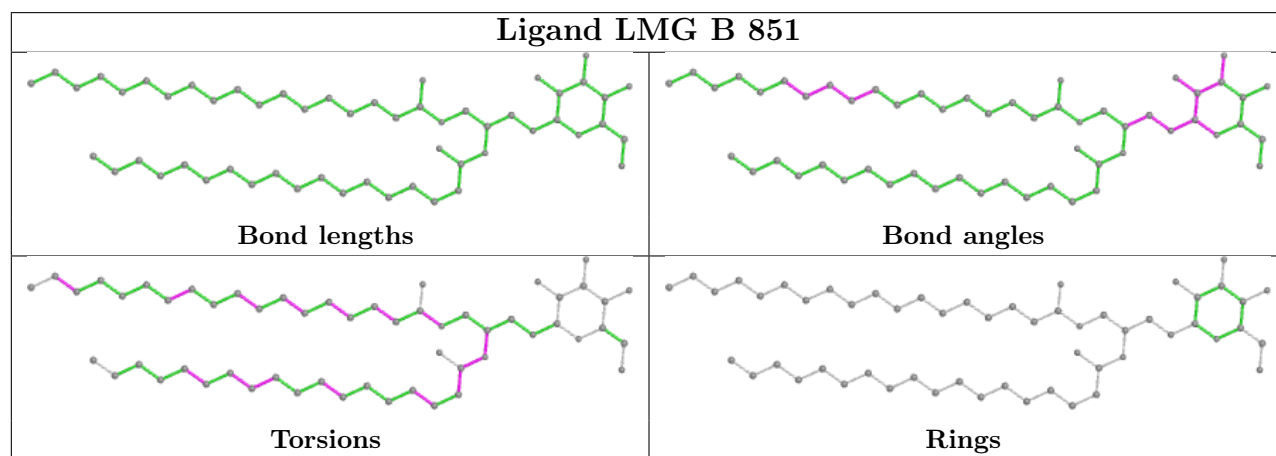


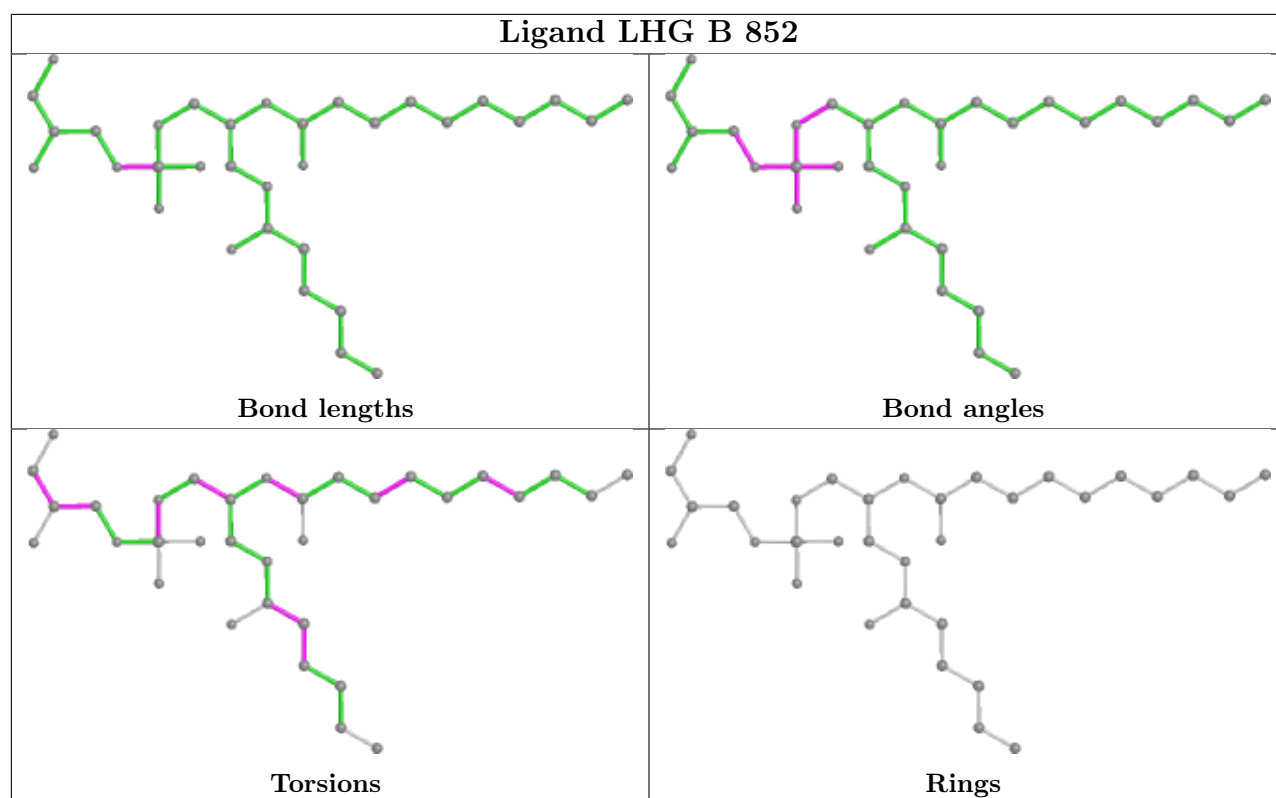
Ligand CLA B 846

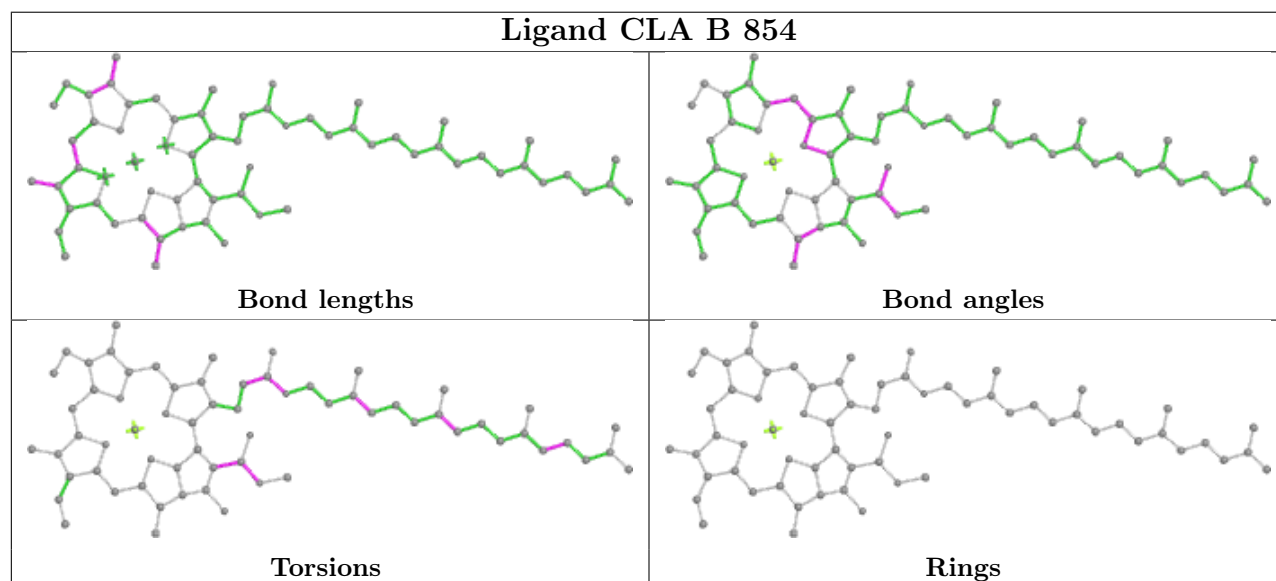
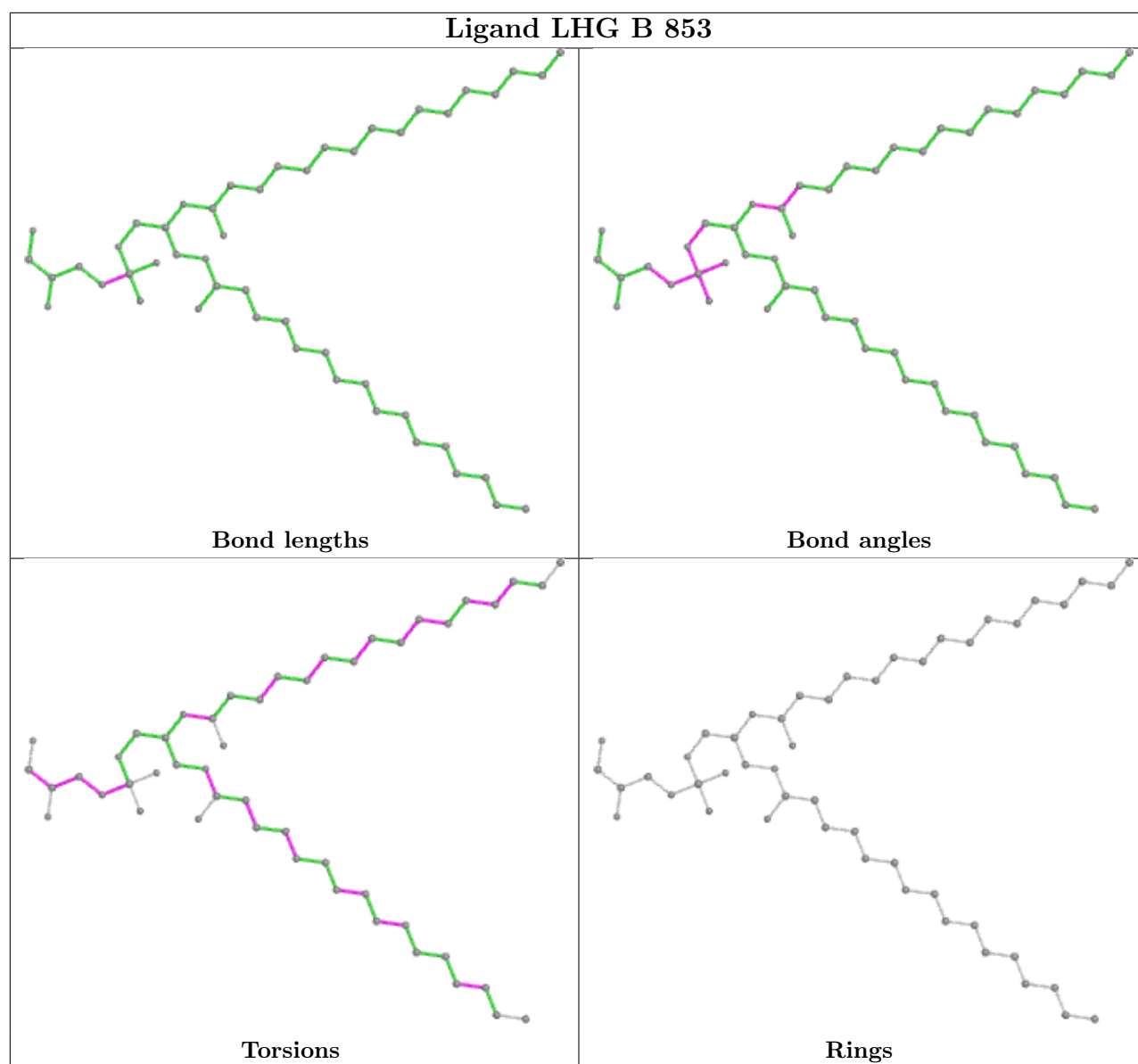


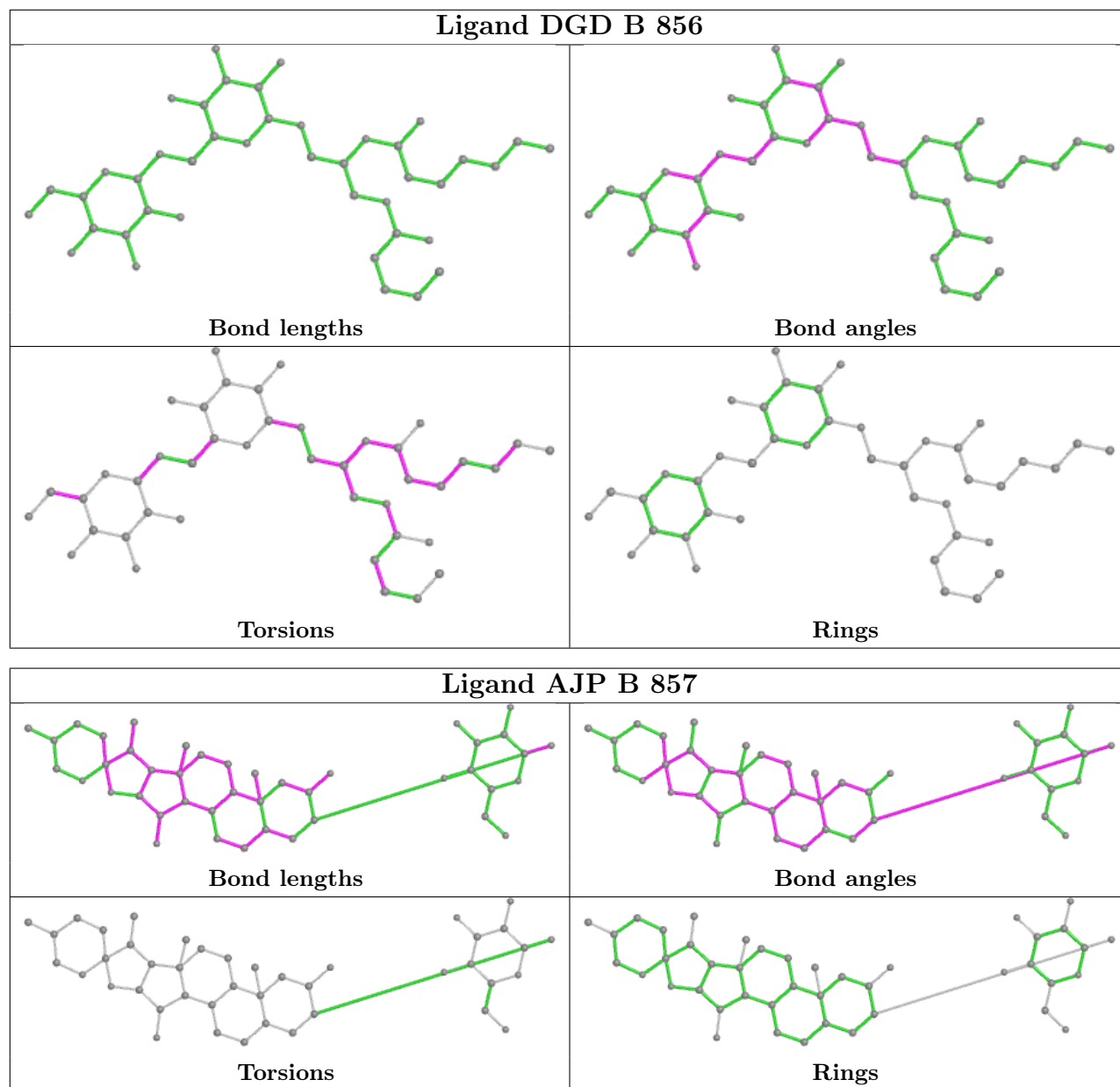
Ligand BCR B 848



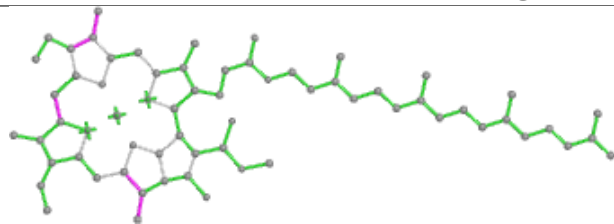
Ligand AJP B 849**Ligand AJP B 850****Ligand LMG B 851**



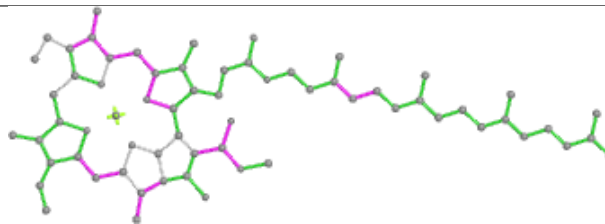




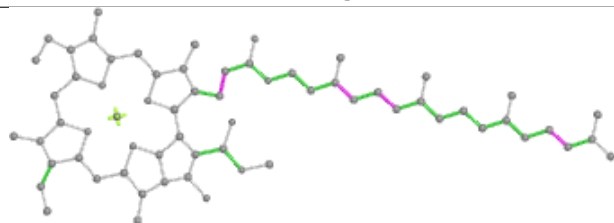
Ligand CLA B 858



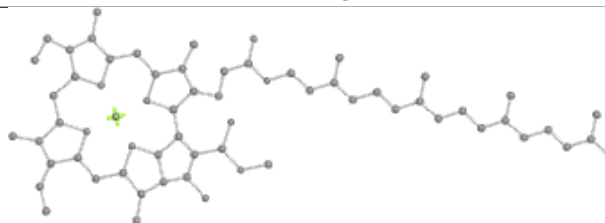
Bond lengths



Bond angles

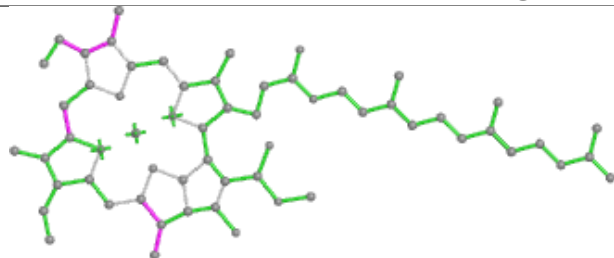


Torsions

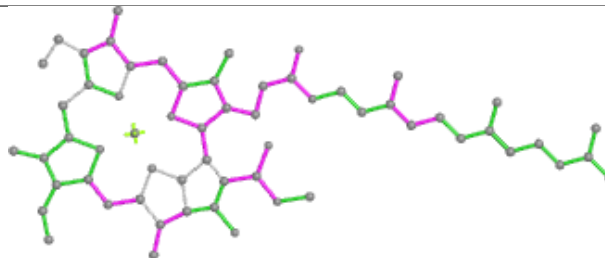


Rings

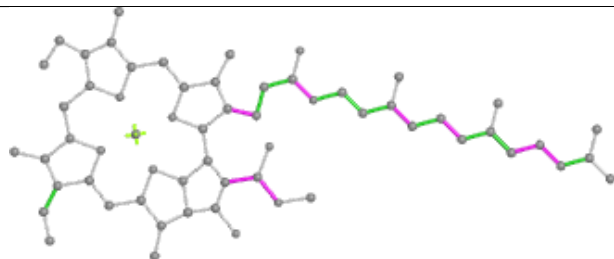
Ligand CLA B 859



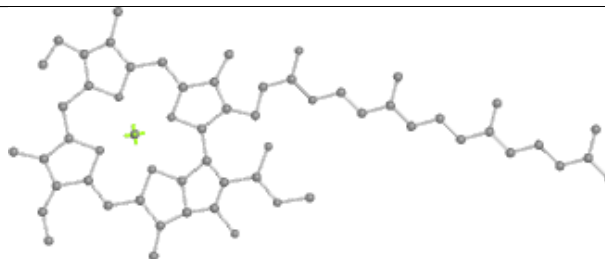
Bond lengths



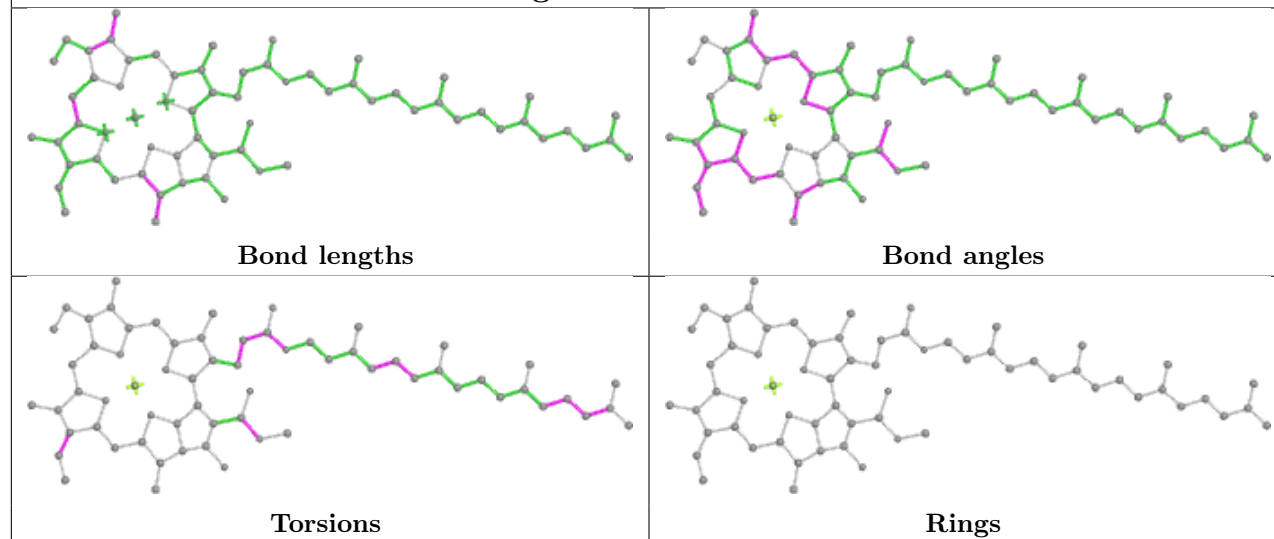
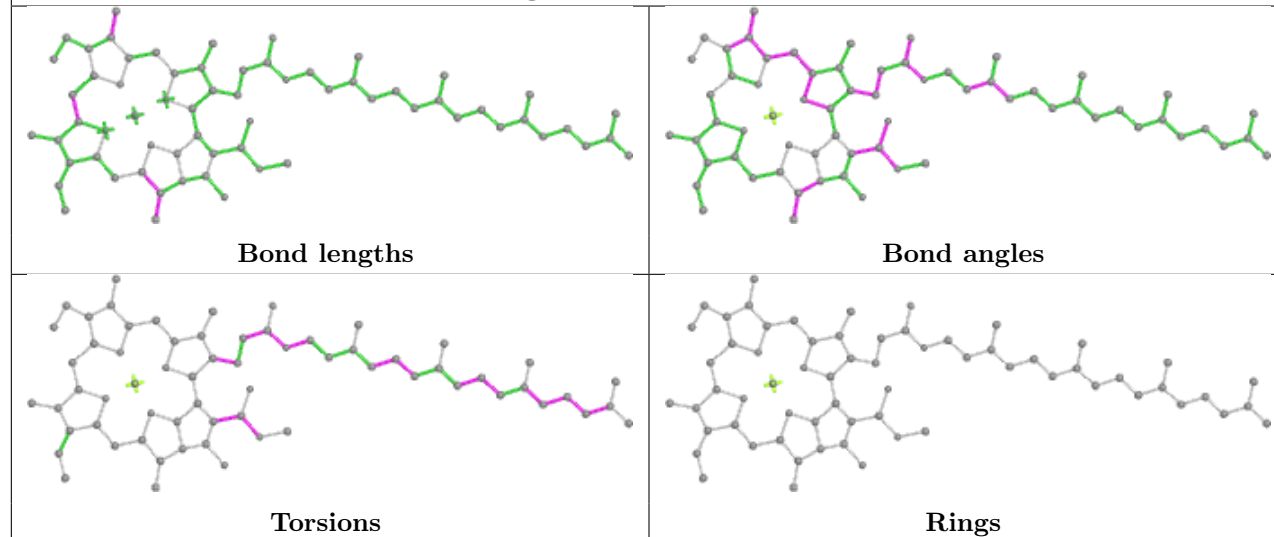
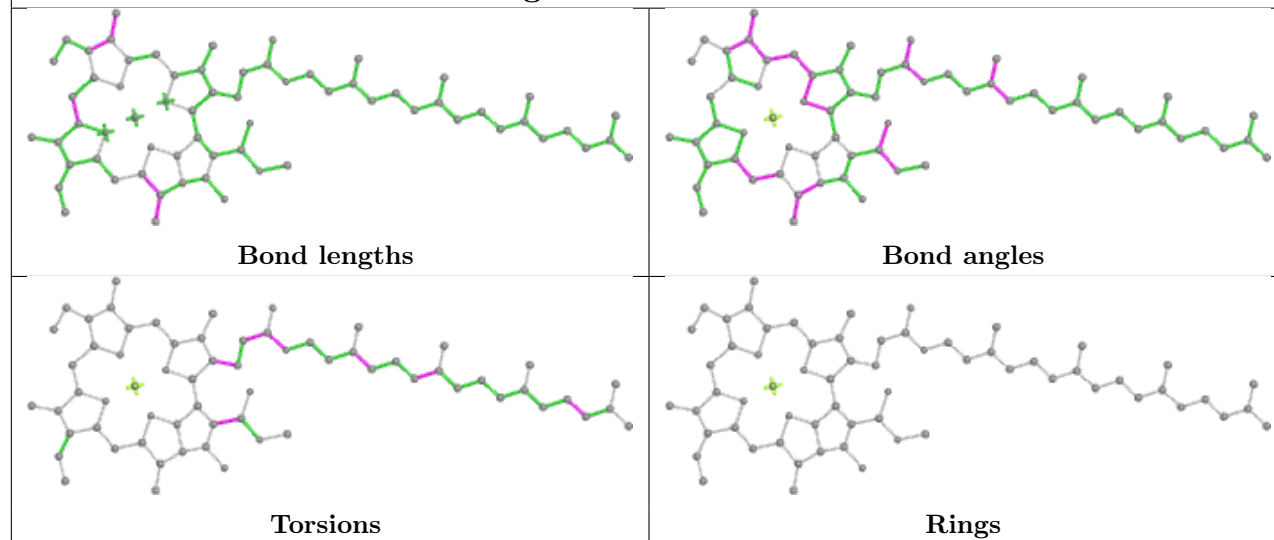
Bond angles

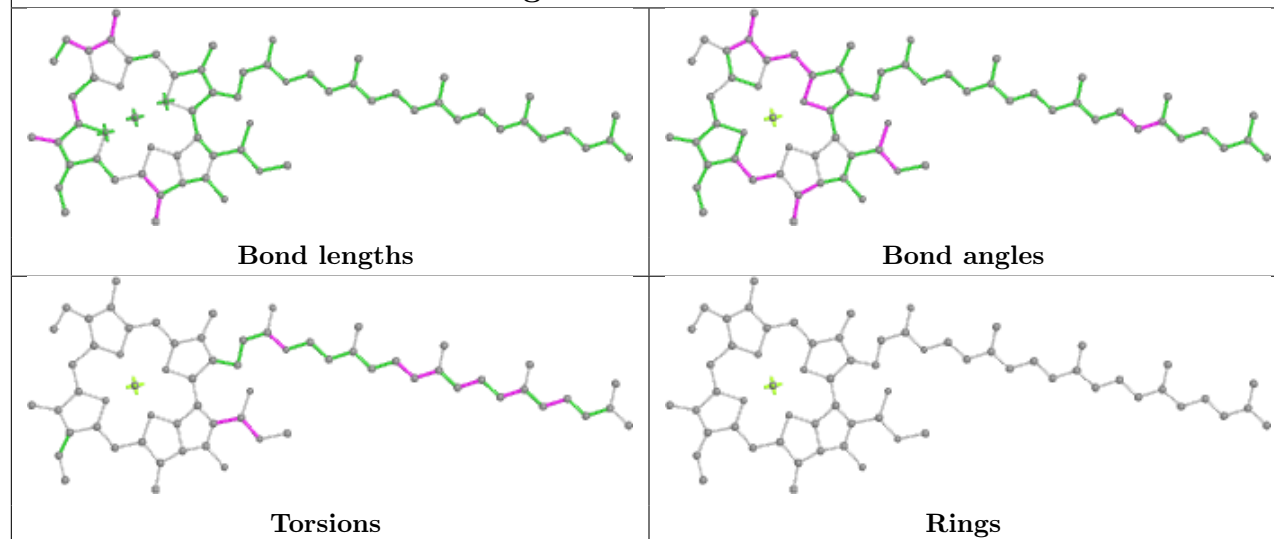
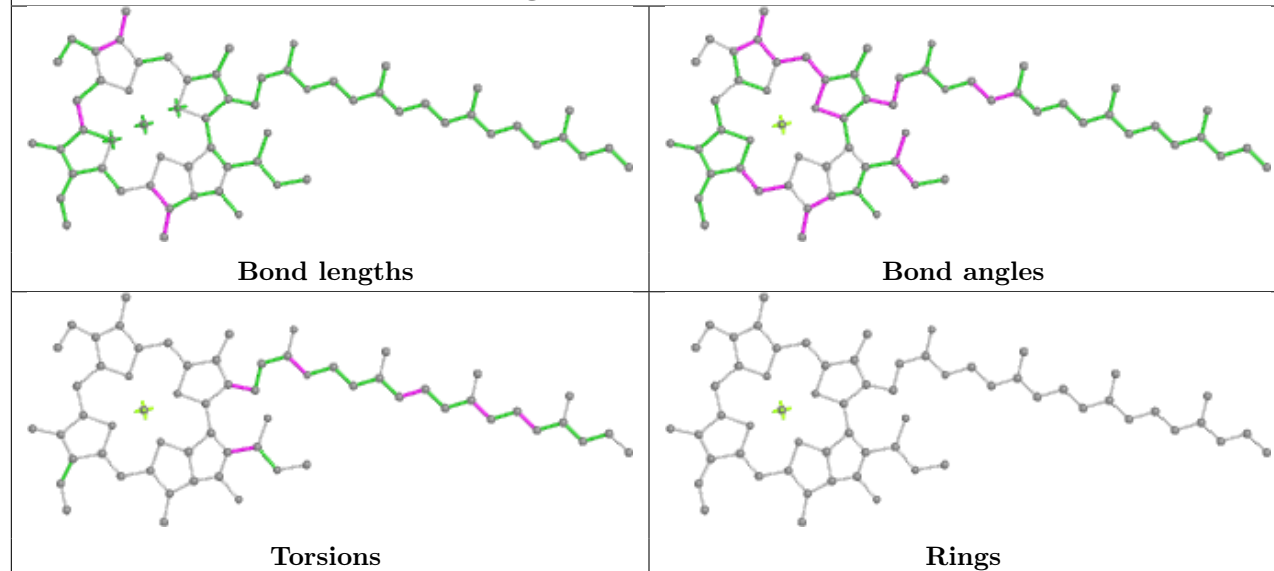


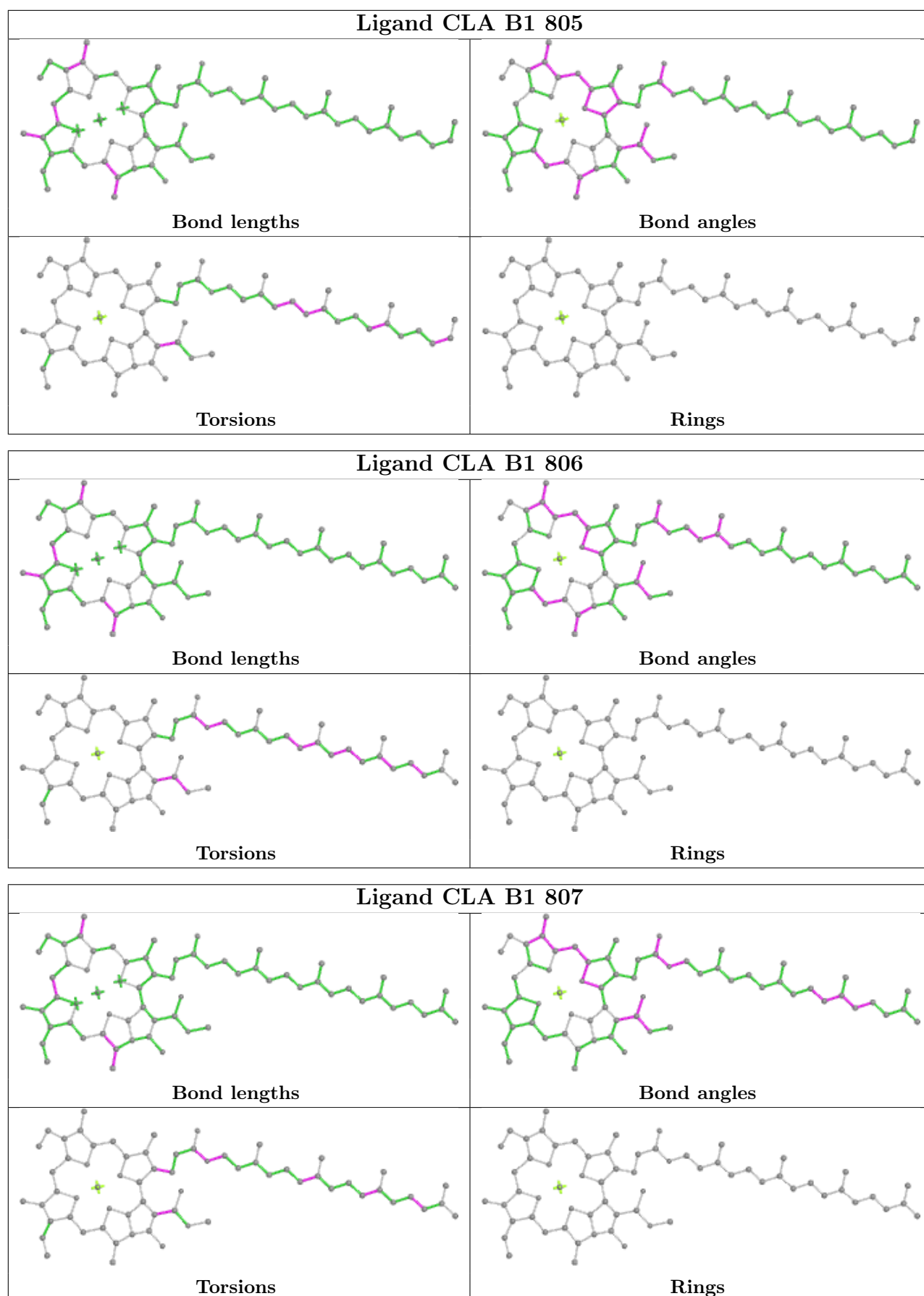
Torsions



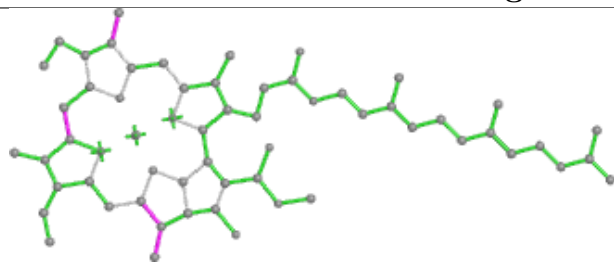
Rings

Ligand CLA B 860**Ligand CLA B1 801****Ligand CLA B1 802**

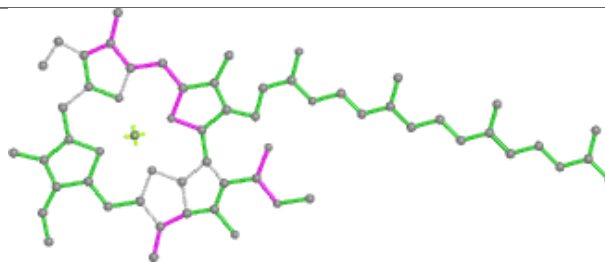
Ligand CLA B1 803**Ligand CLA B1 804**



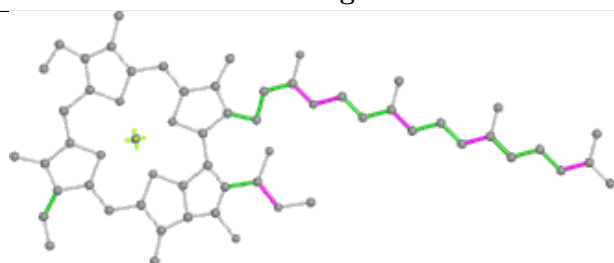
Ligand CLA B1 808



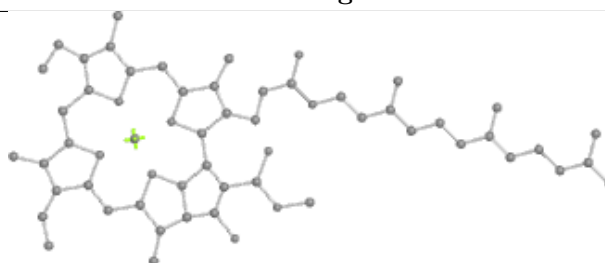
Bond lengths



Bond angles

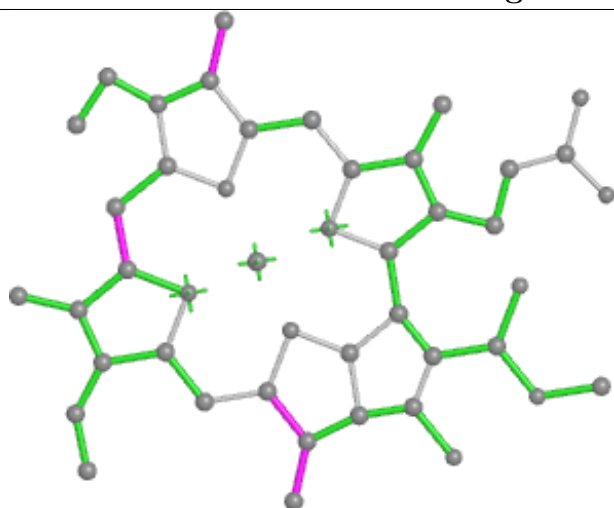


Torsions

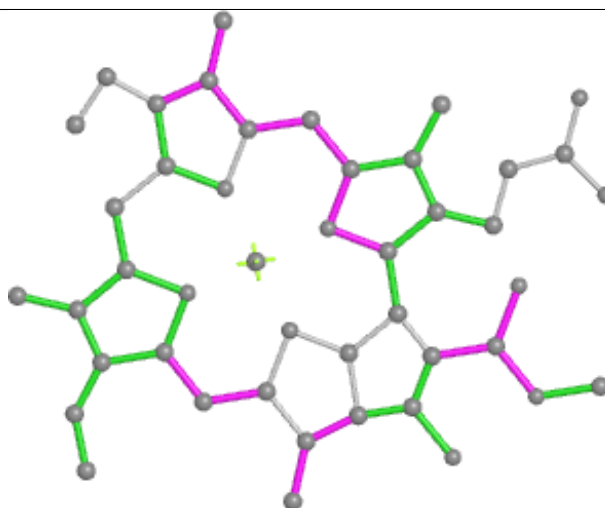


Rings

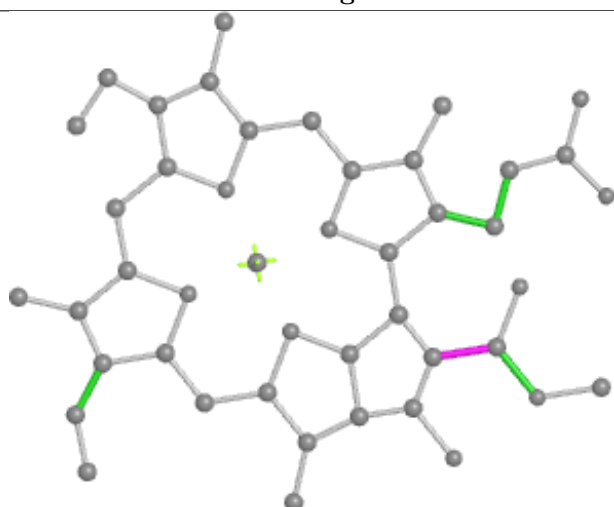
Ligand CLA B1 809



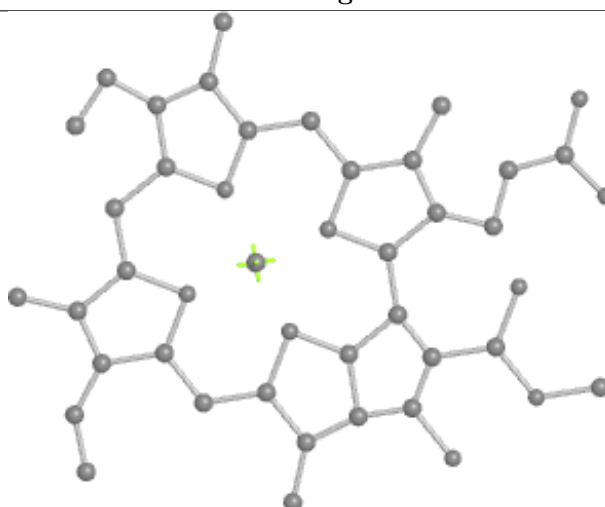
Bond lengths



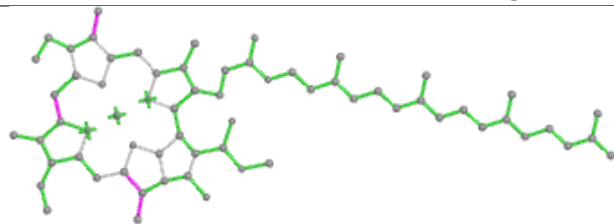
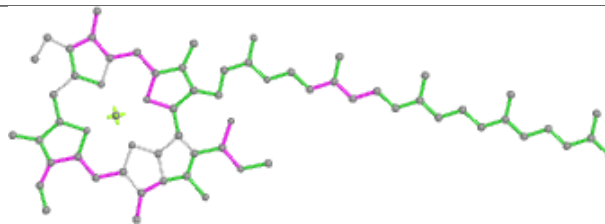
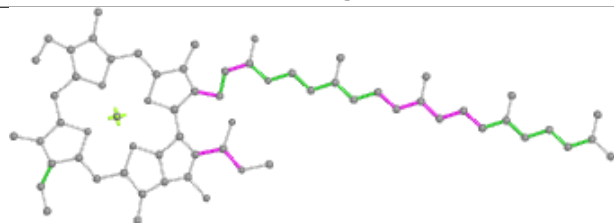
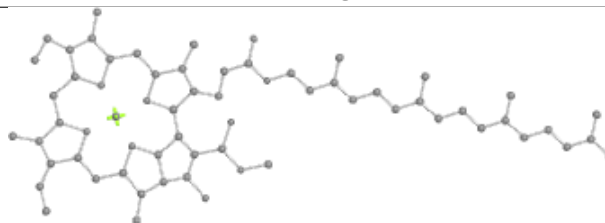
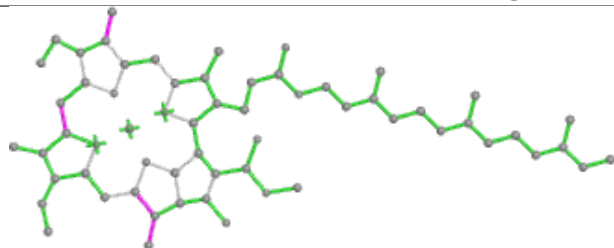
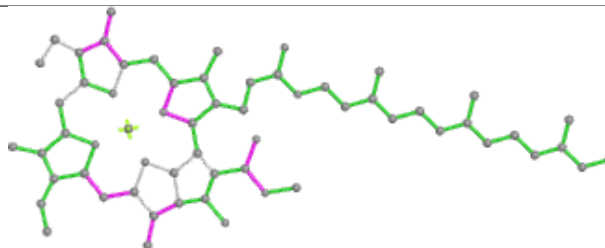
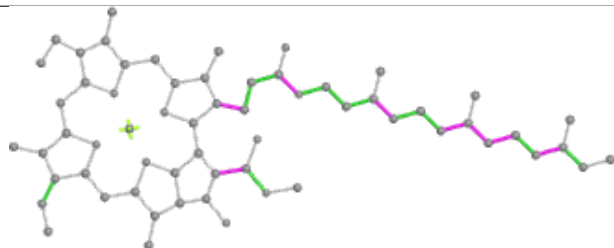
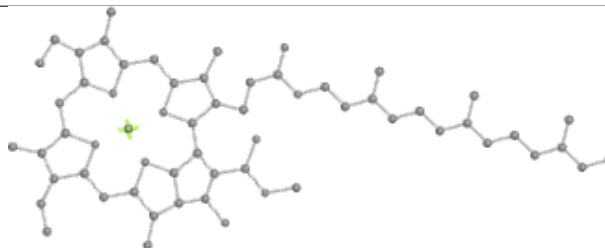
Bond angles



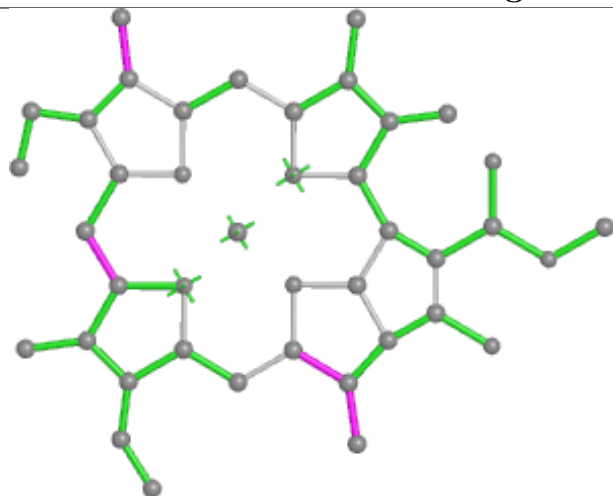
Torsions



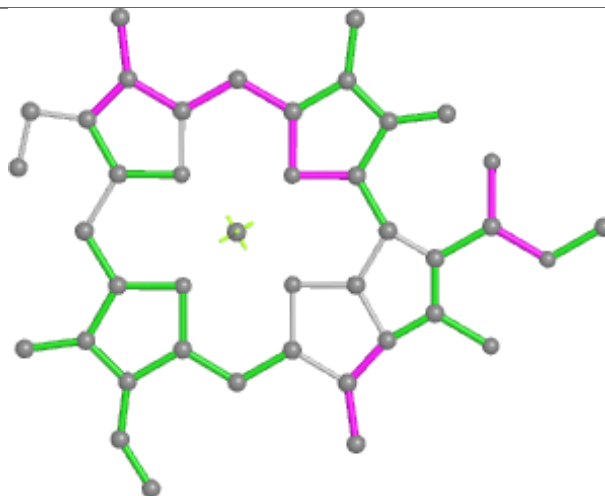
Rings

Ligand CLA B1 810**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B1 811****Bond lengths****Bond angles****Torsions****Rings**

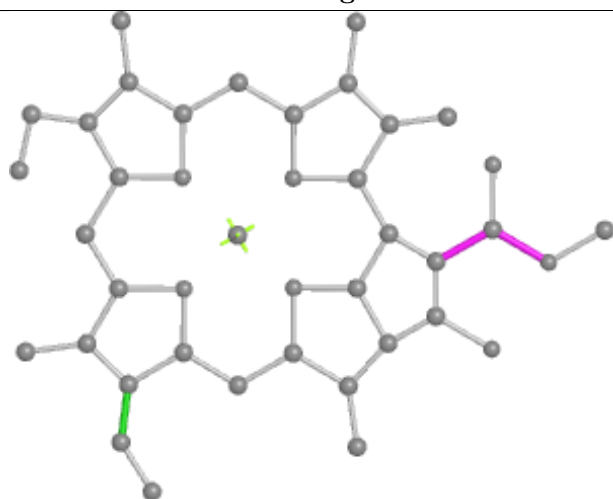
Ligand CLA B1 812



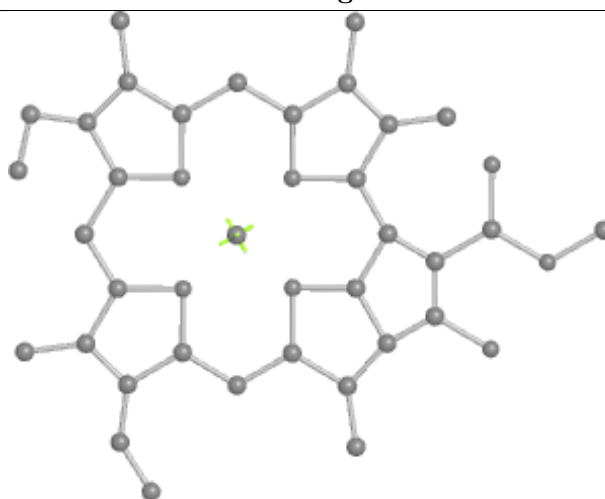
Bond lengths



Bond angles

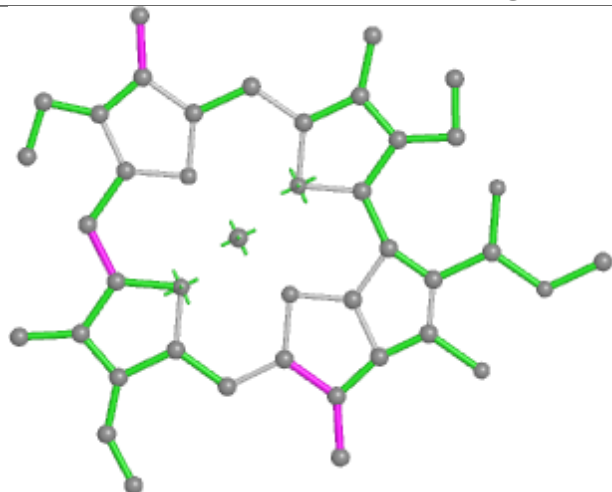


Torsions

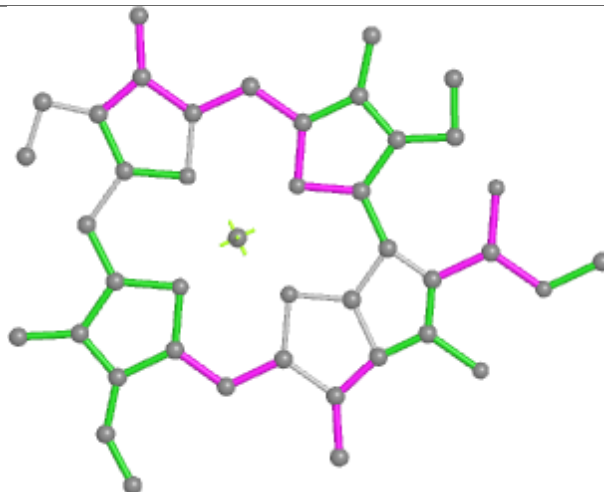


Rings

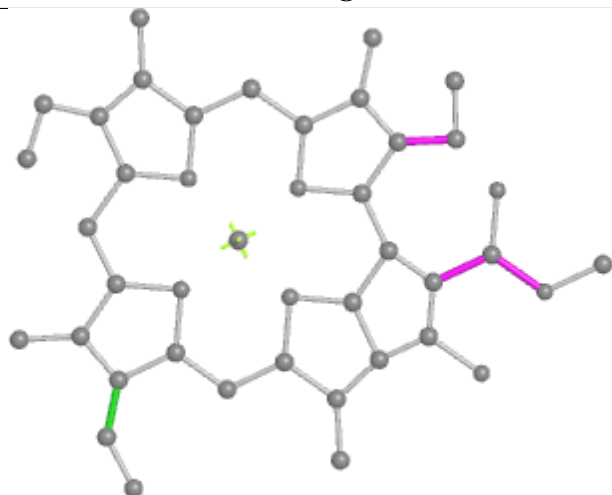
Ligand CLA B1 813



Bond lengths



Bond angles

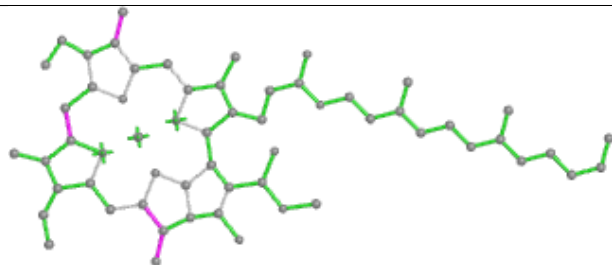


Torsions

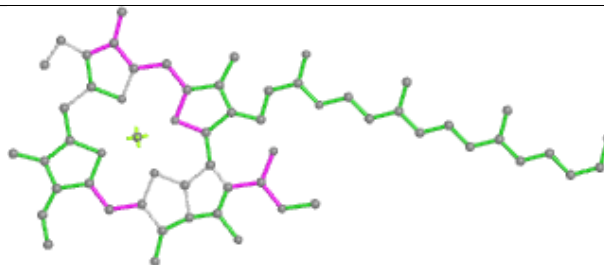


Rings

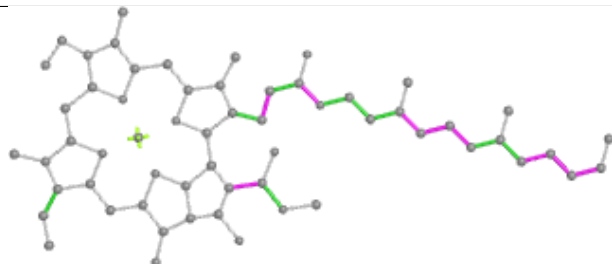
Ligand CLA B1 814



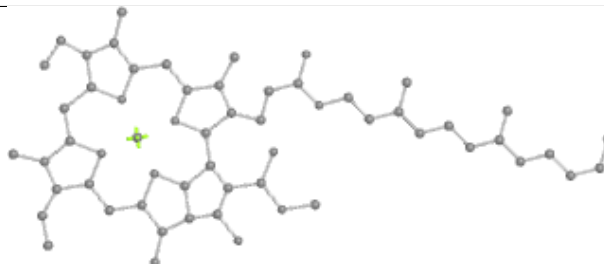
Bond lengths



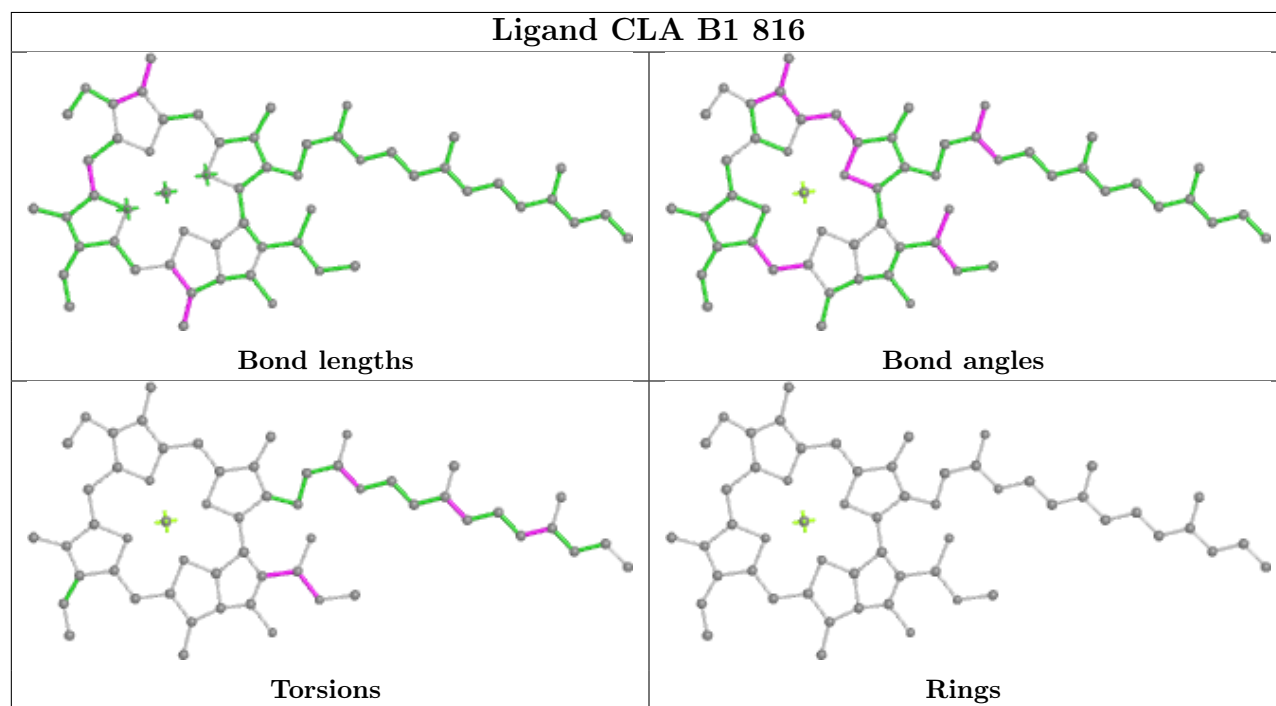
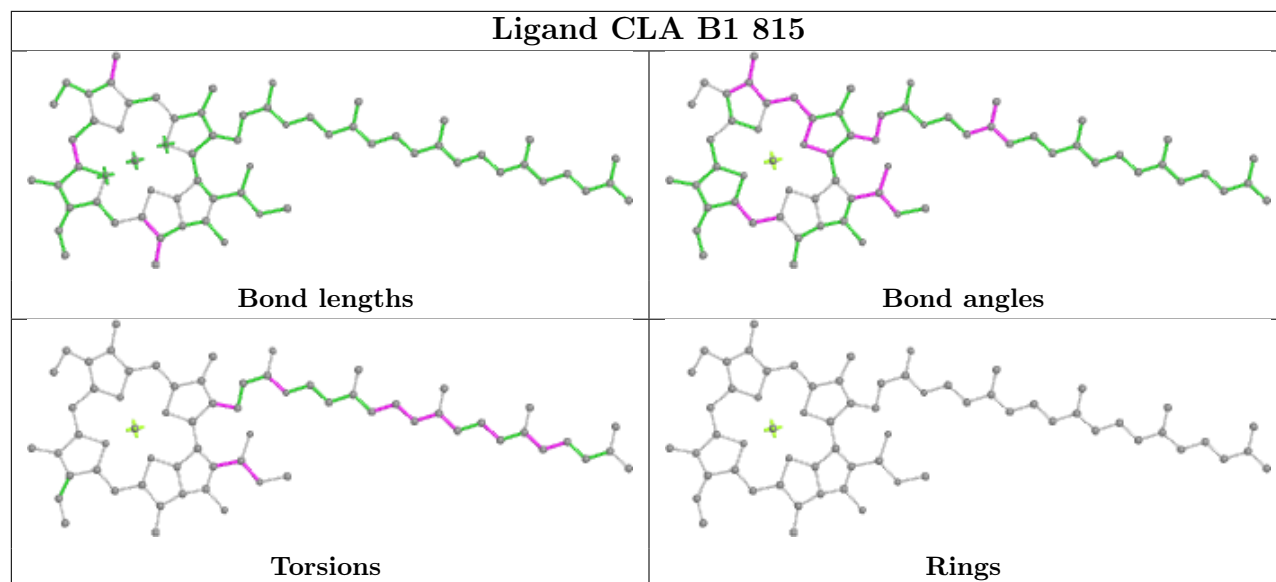
Bond angles



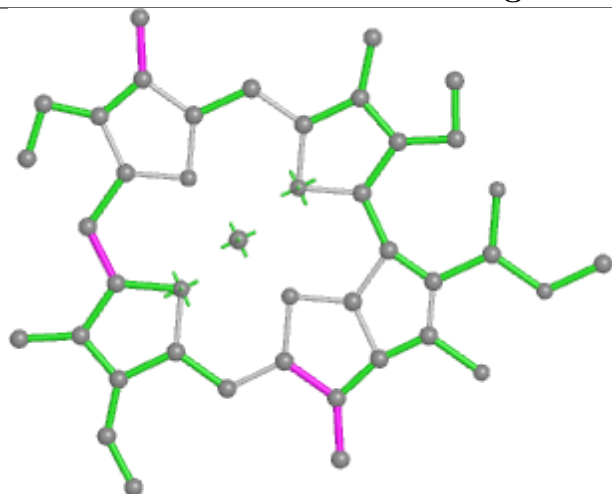
Torsions



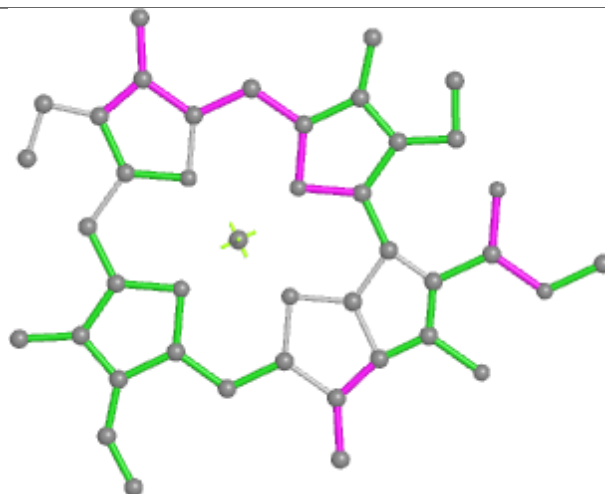
Rings



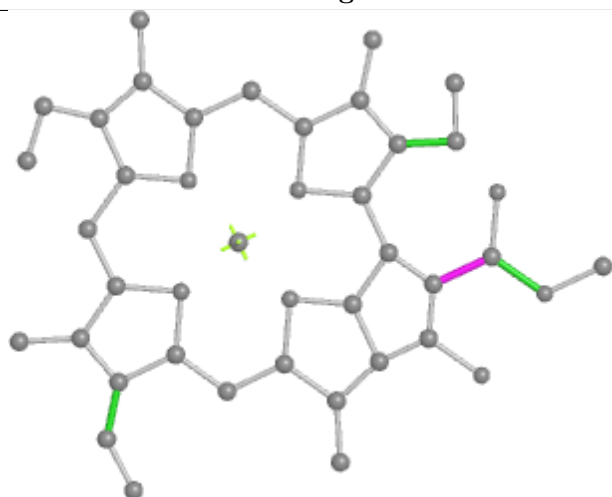
Ligand CLA B1 817



Bond lengths



Bond angles

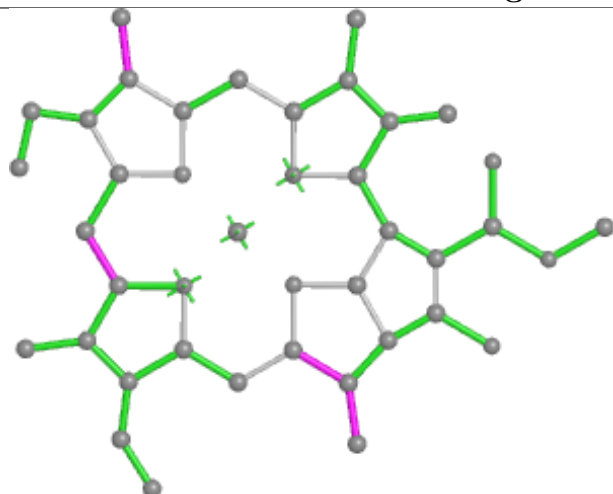


Torsions

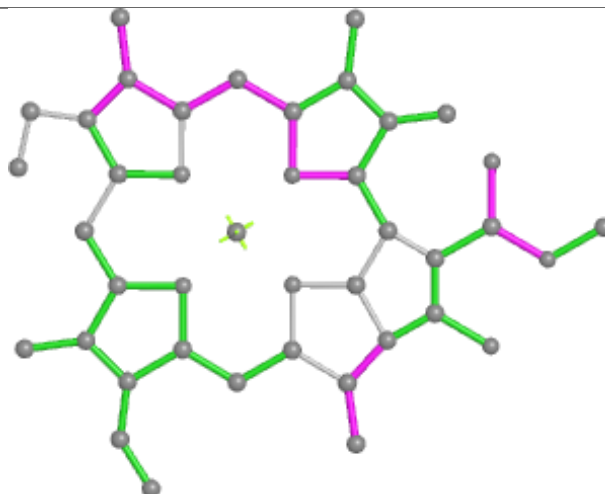


Rings

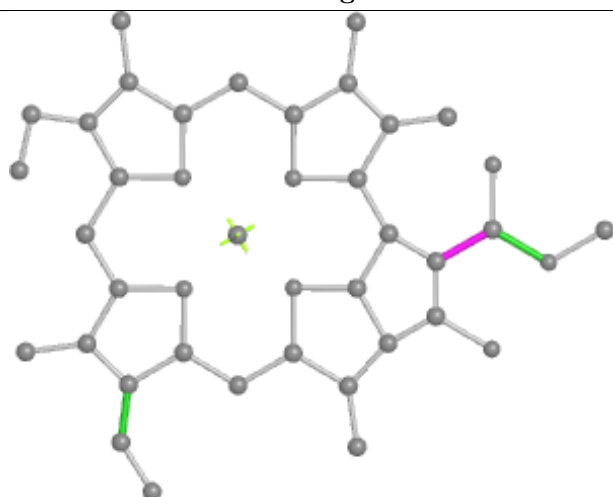
Ligand CLA B1 818



Bond lengths



Bond angles

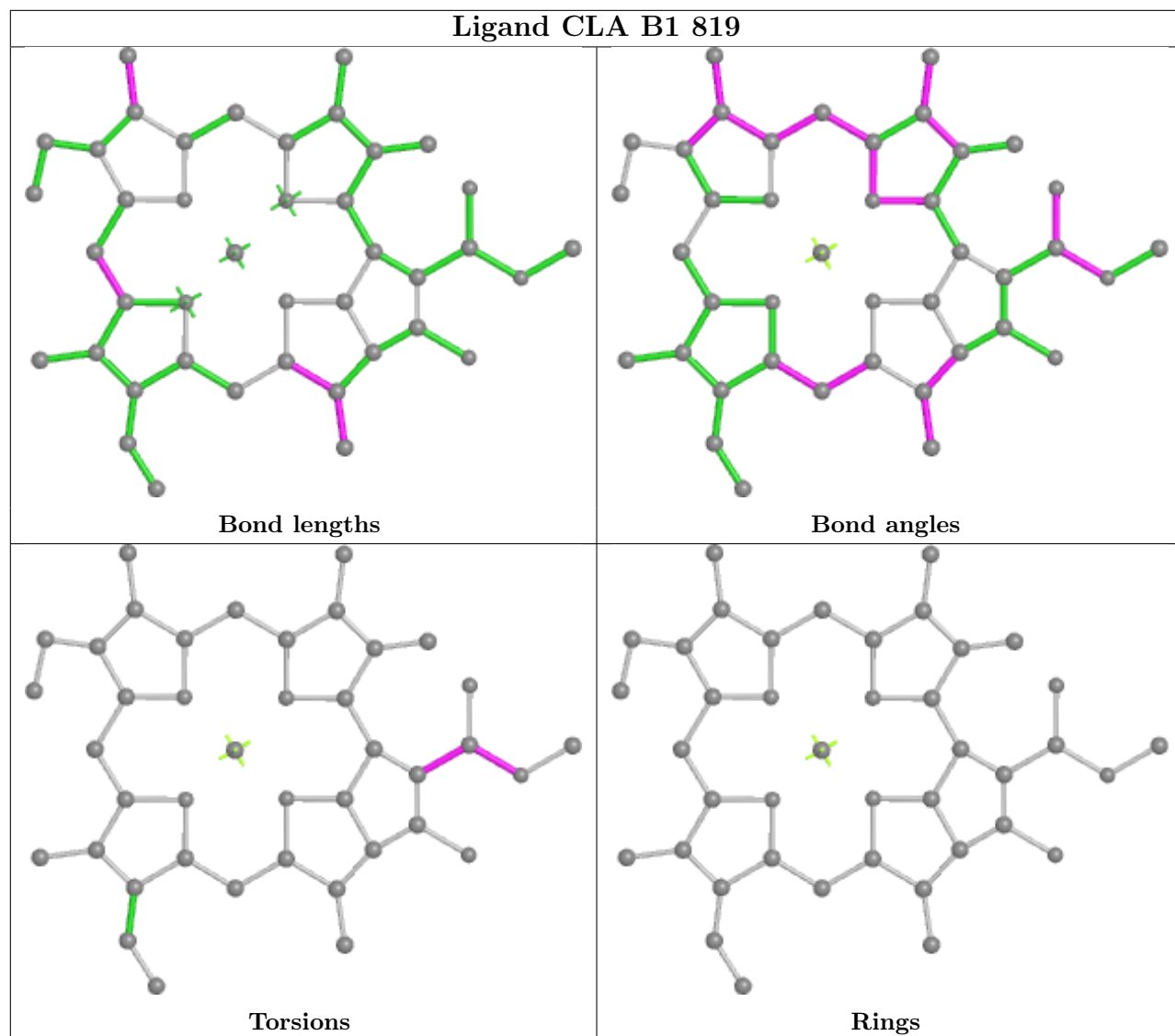


Torsions

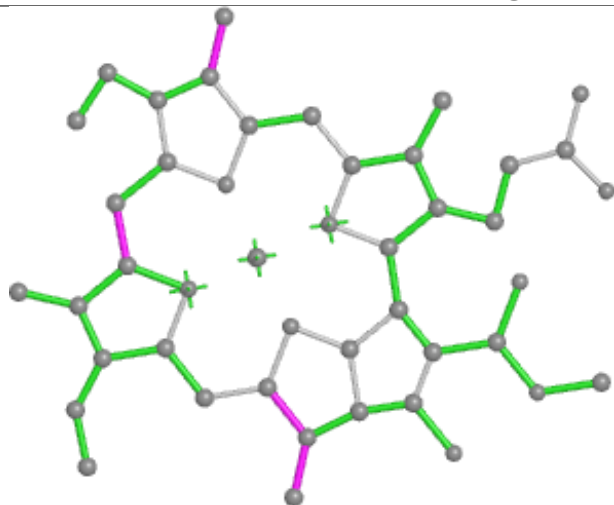


Rings

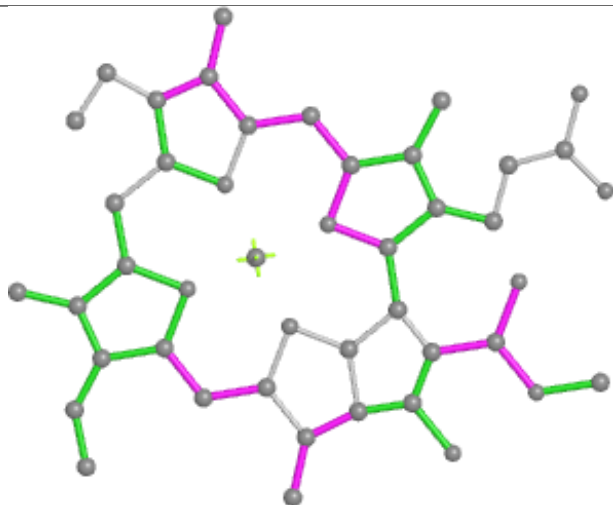
Ligand CLA B1 819



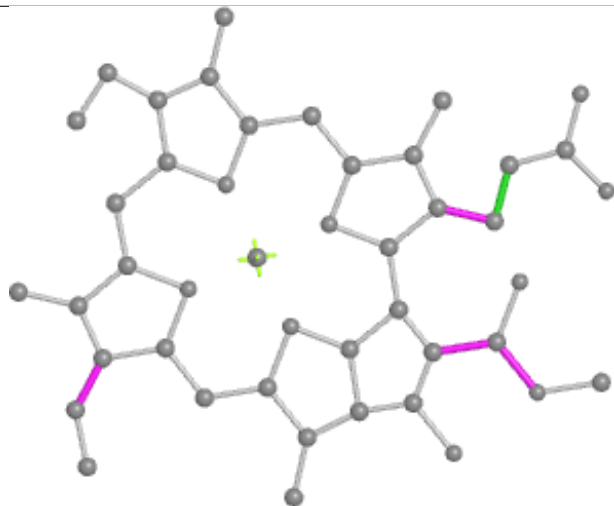
Ligand CLA B1 820



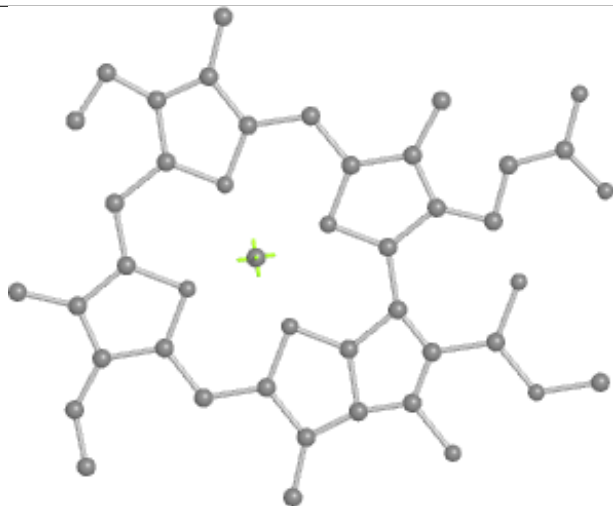
Bond lengths



Bond angles

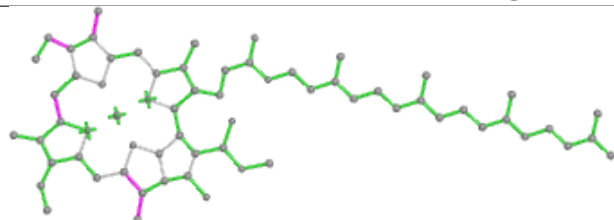


Torsions

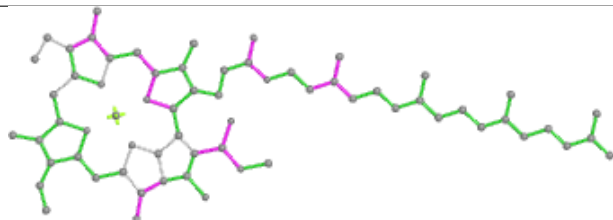


Rings

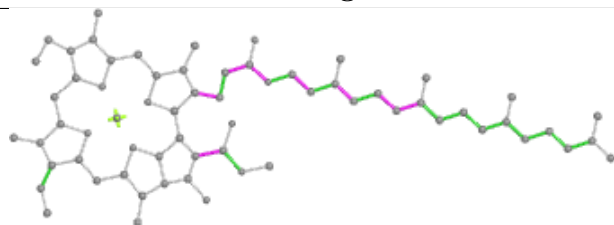
Ligand CLA B1 821



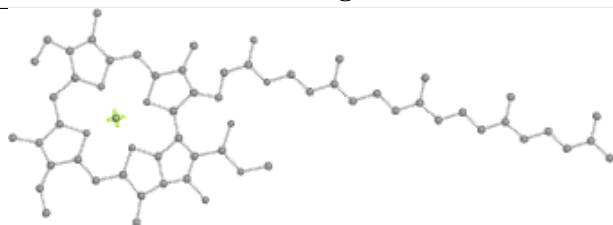
Bond lengths



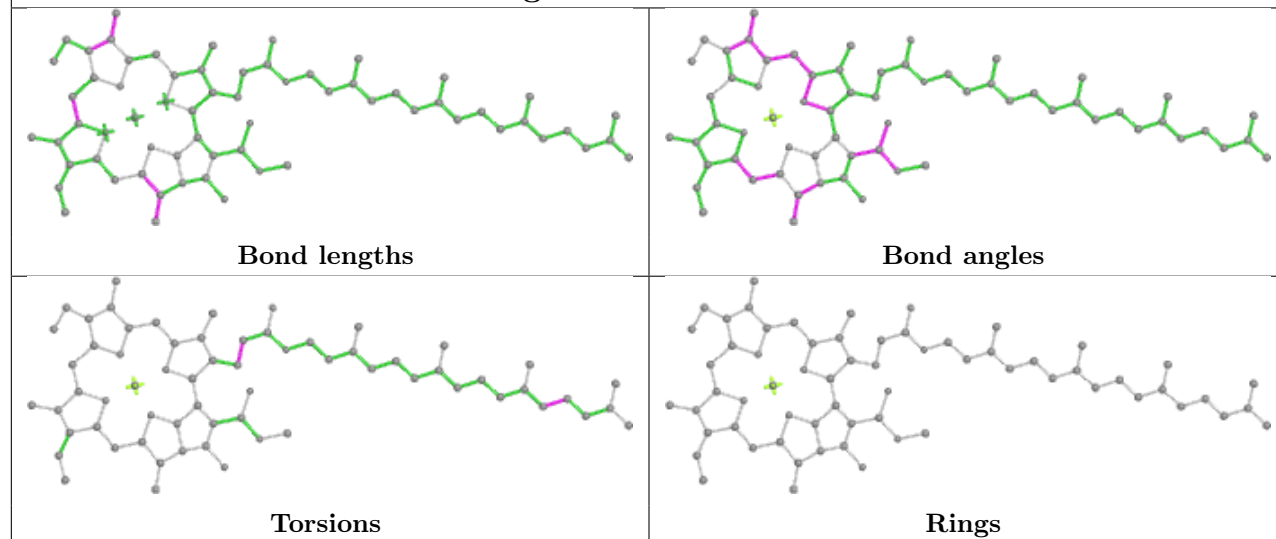
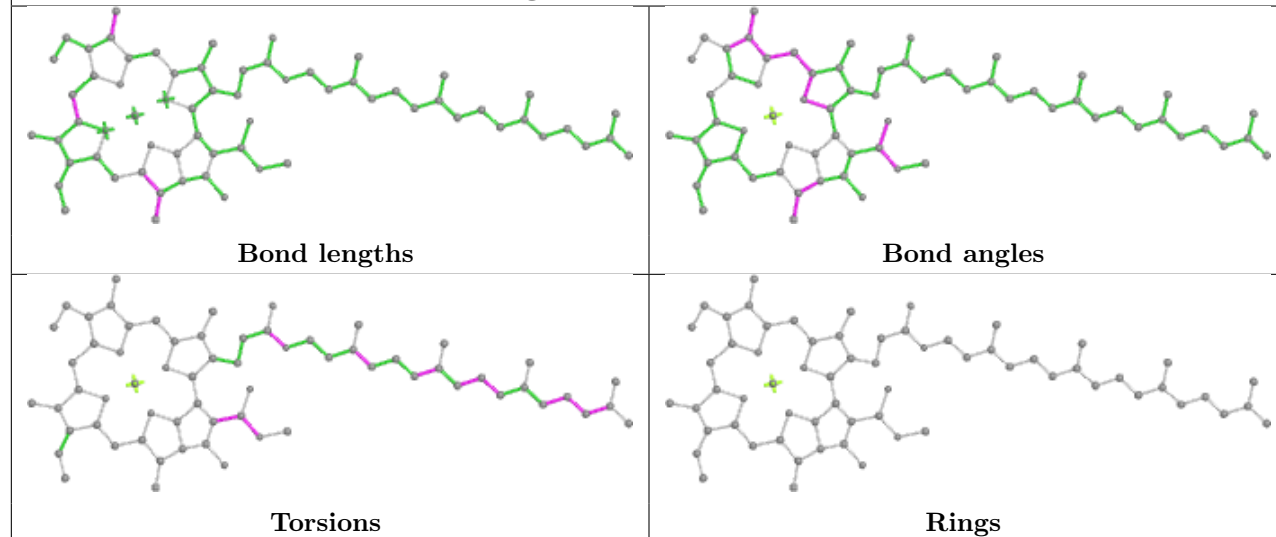
Bond angles



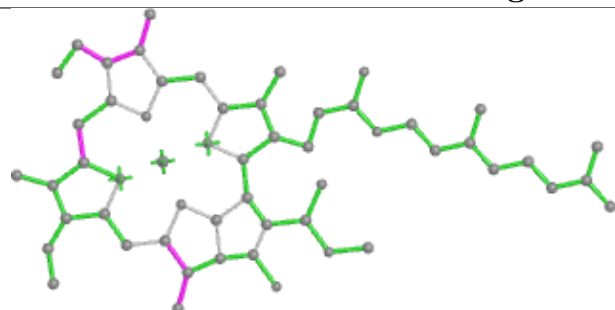
Torsions



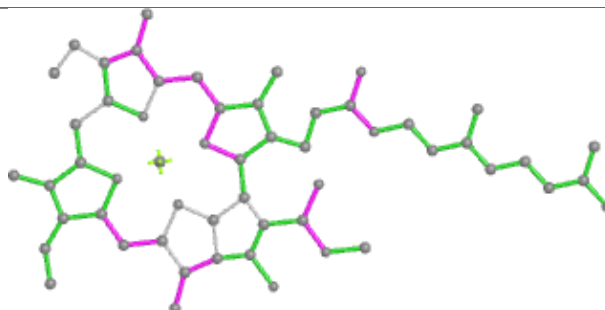
Rings

Ligand CLA B1 822**Ligand CLA B1 823**

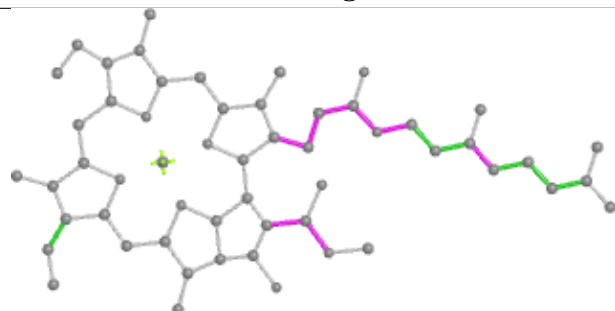
Ligand CLA B1 824



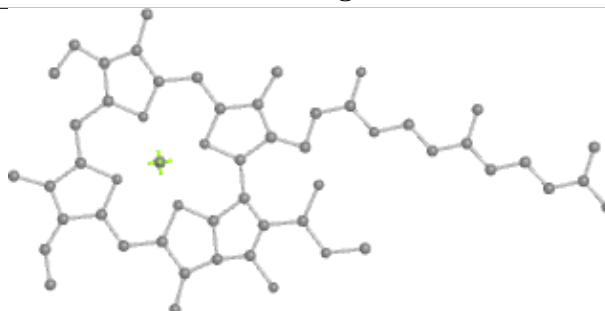
Bond lengths



Bond angles

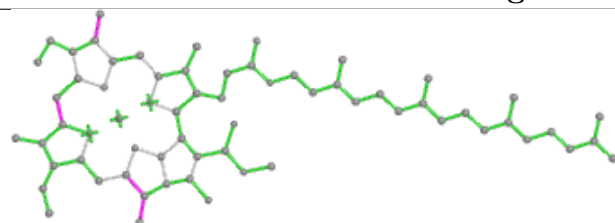


Torsions

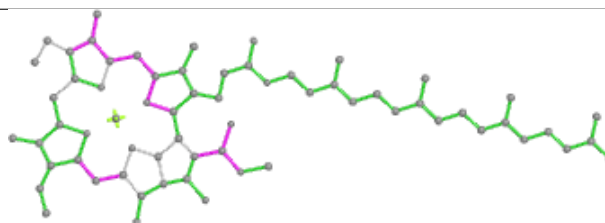


Rings

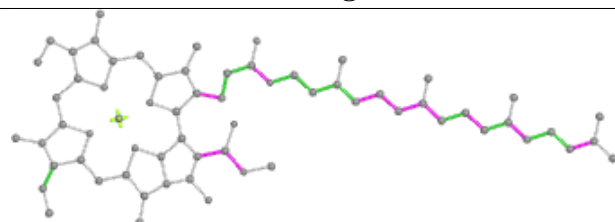
Ligand CLA B1 825



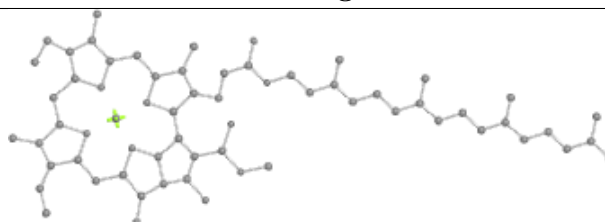
Bond lengths



Bond angles

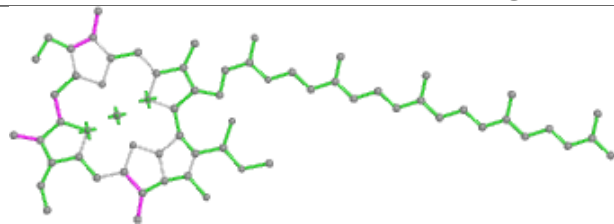


Torsions

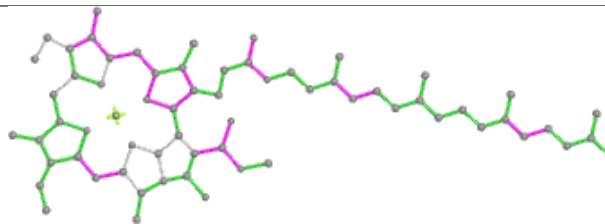


Rings

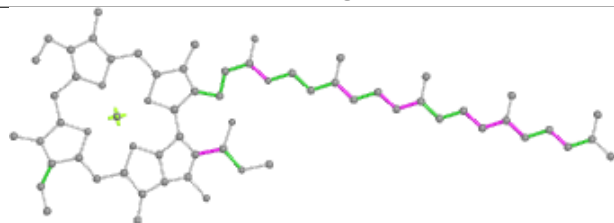
Ligand CLA B1 826



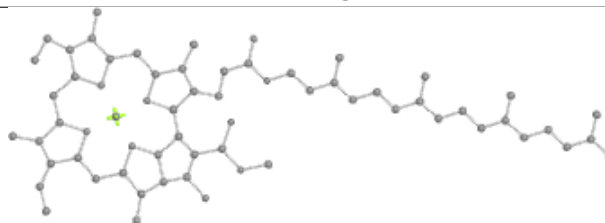
Bond lengths



Bond angles

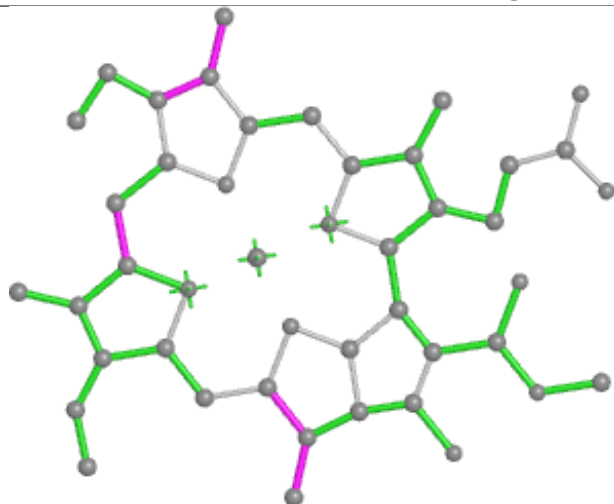


Torsions

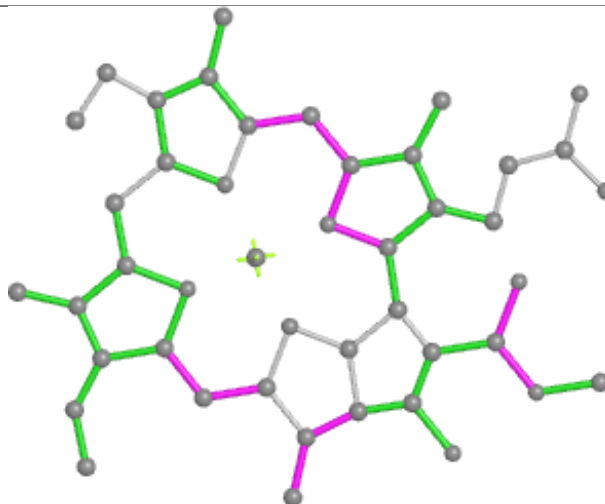


Rings

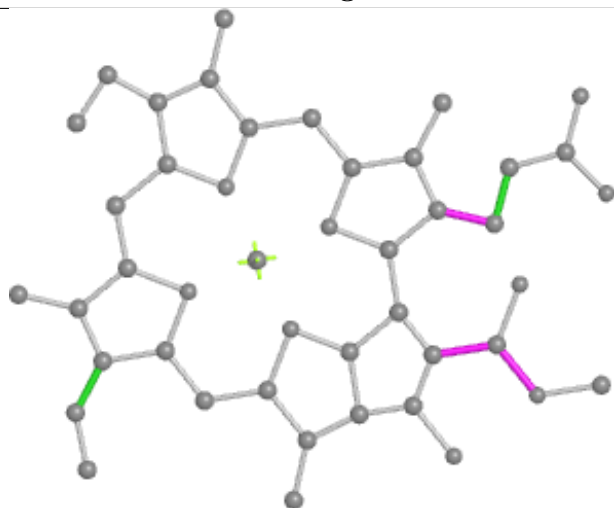
Ligand CLA B1 827



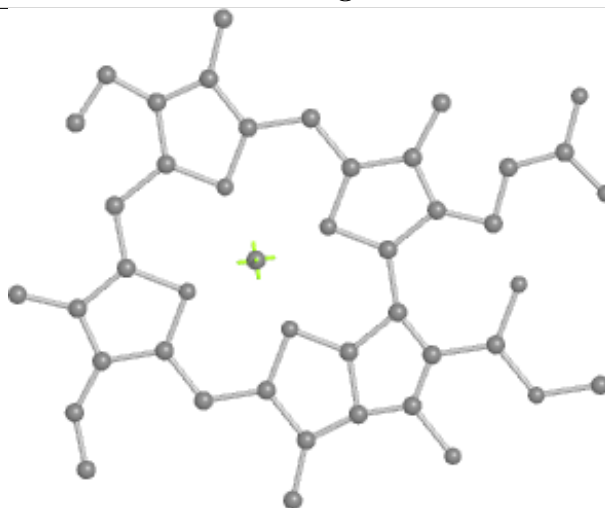
Bond lengths



Bond angles

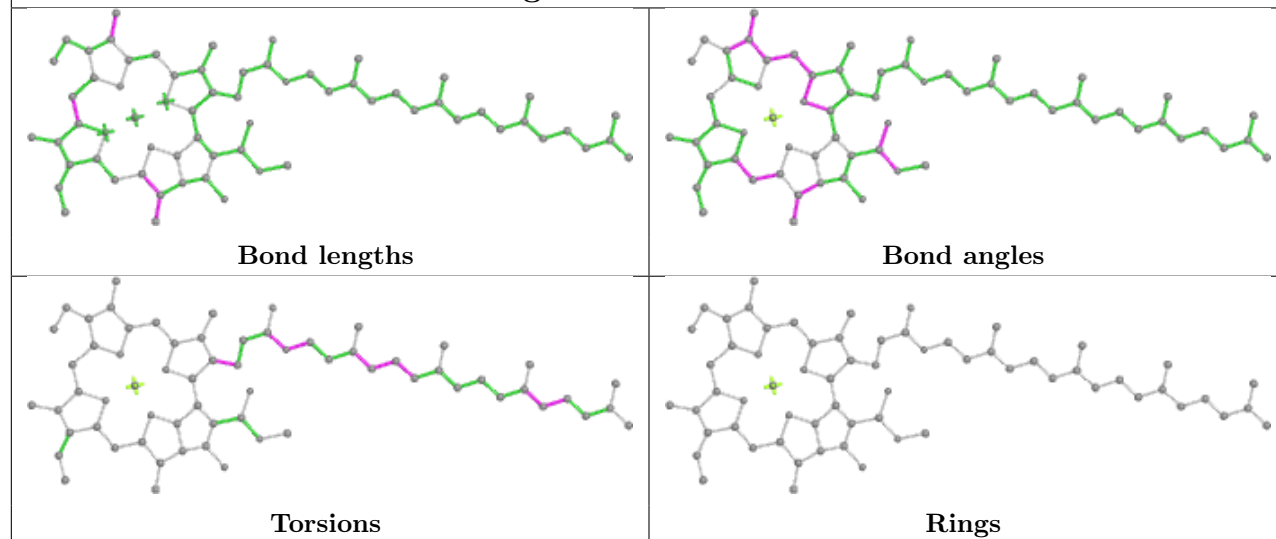


Torsions

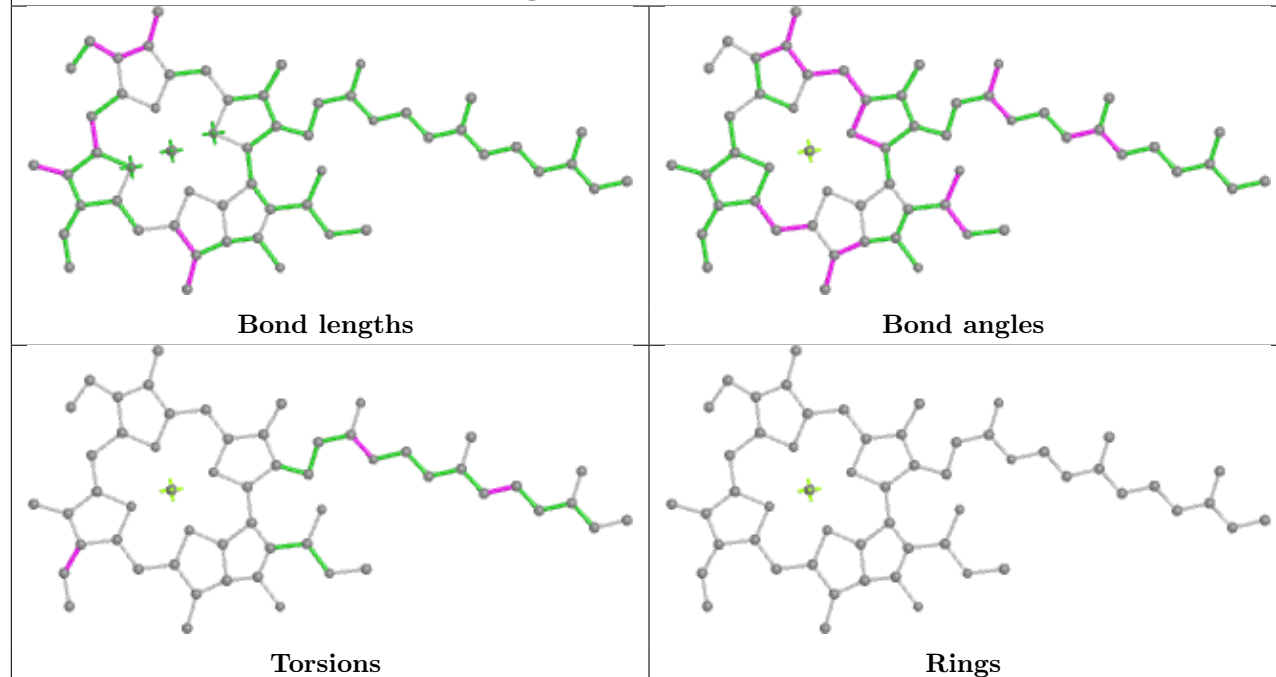


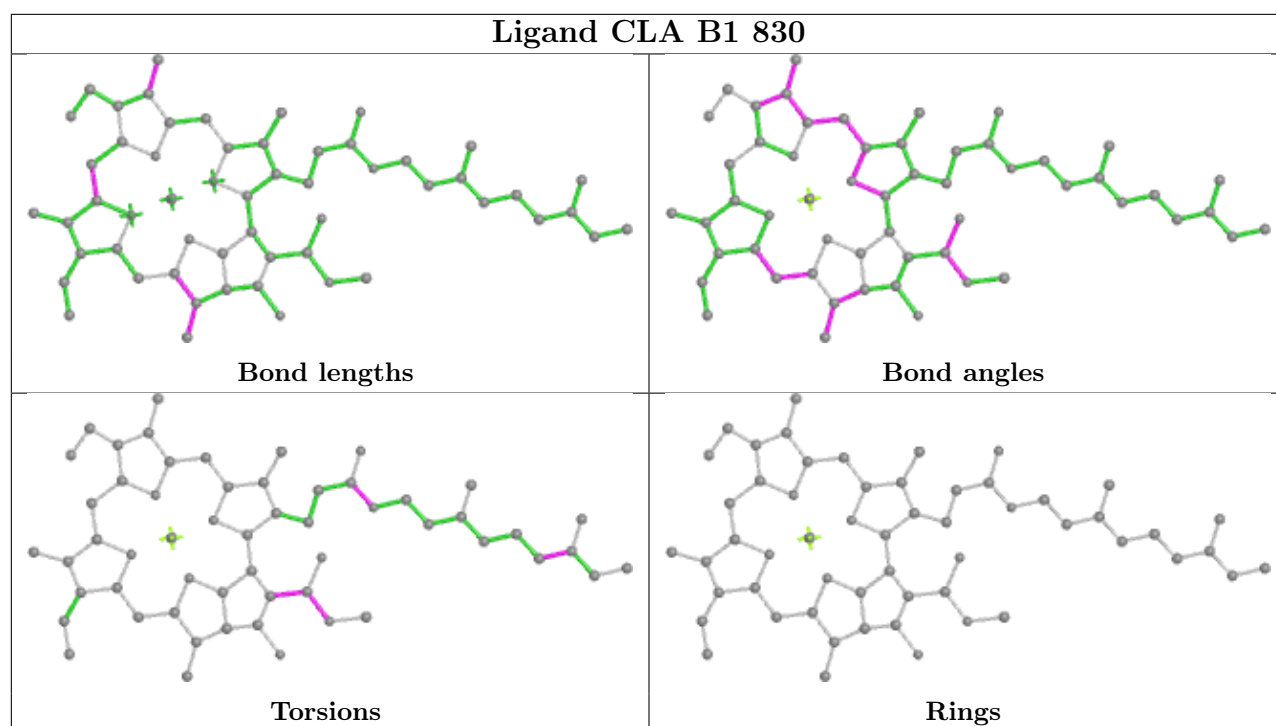
Rings

Ligand CLA B1 828

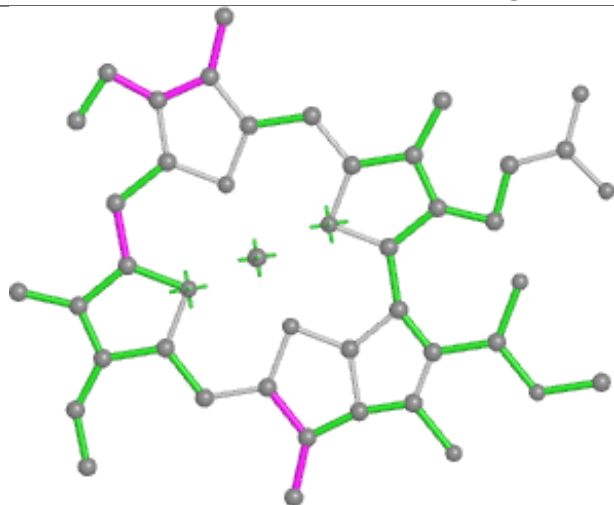


Ligand CLA B1 829

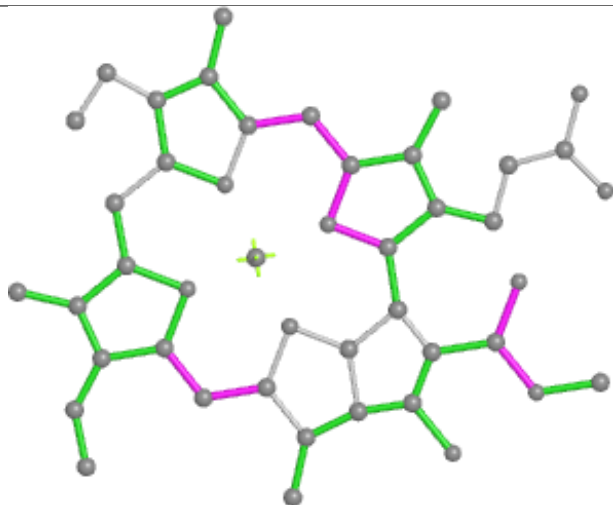




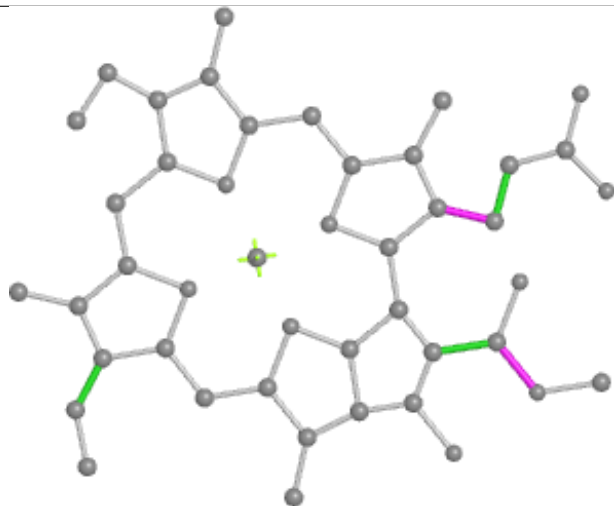
Ligand CLA B1 831



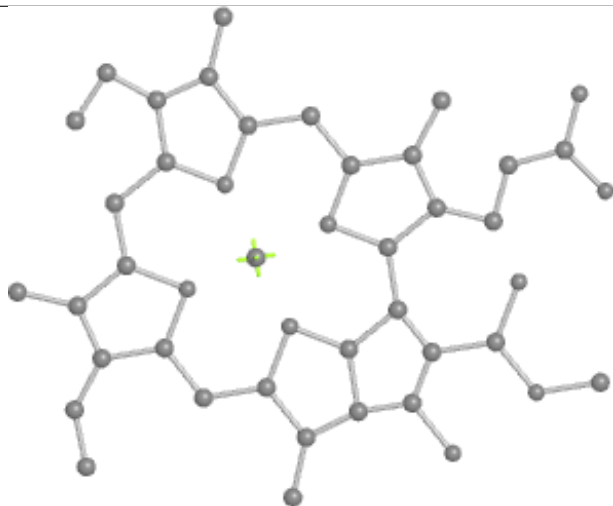
Bond lengths



Bond angles

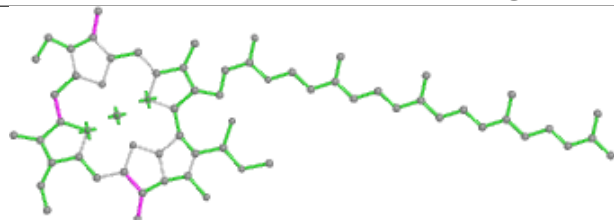


Torsions

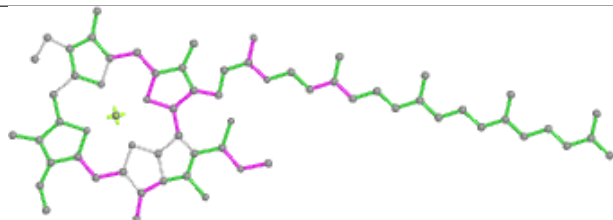


Rings

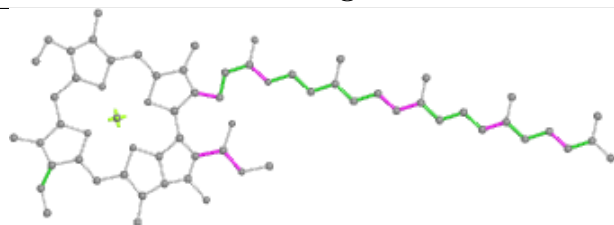
Ligand CLA B1 832



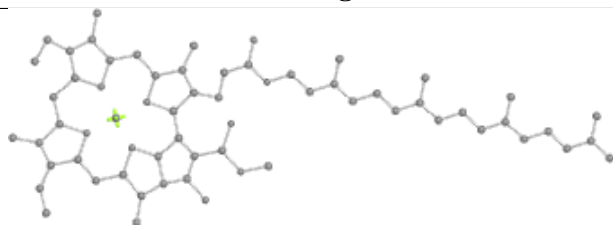
Bond lengths



Bond angles

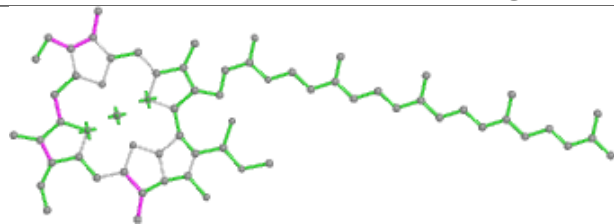


Torsions

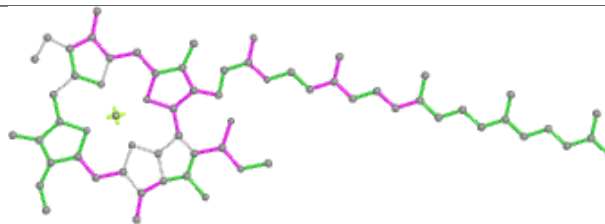


Rings

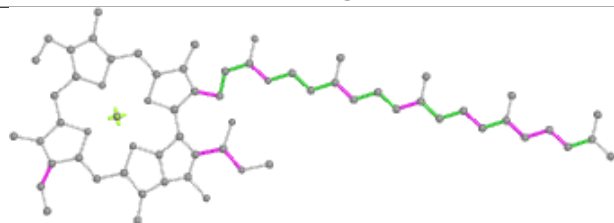
Ligand CLA B1 833



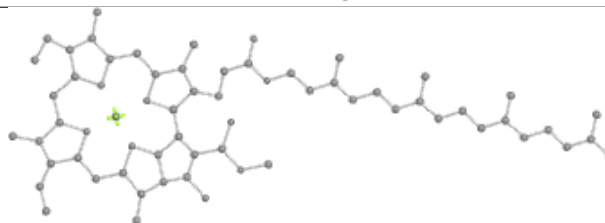
Bond lengths



Bond angles

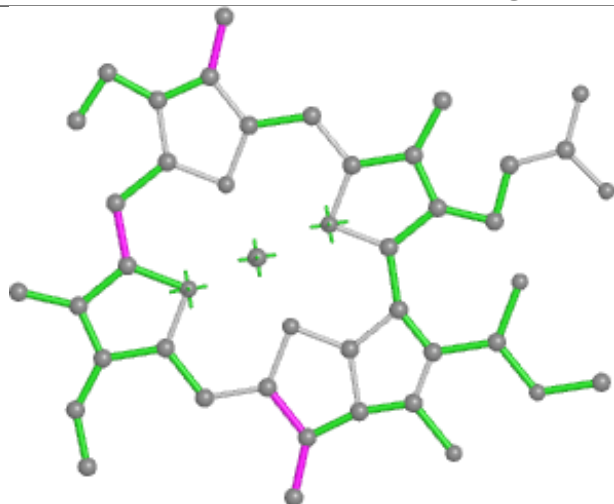


Torsions

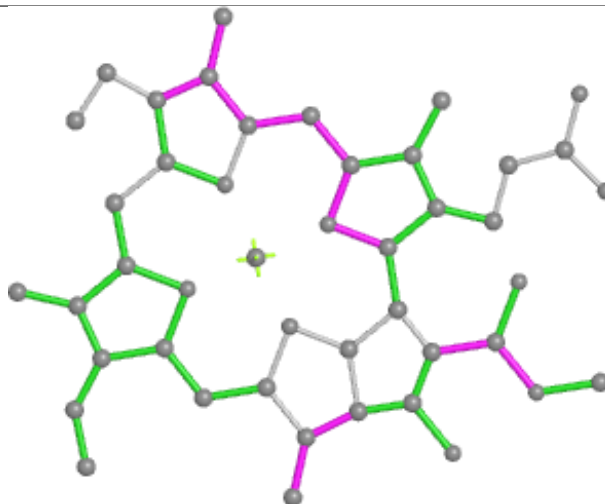


Rings

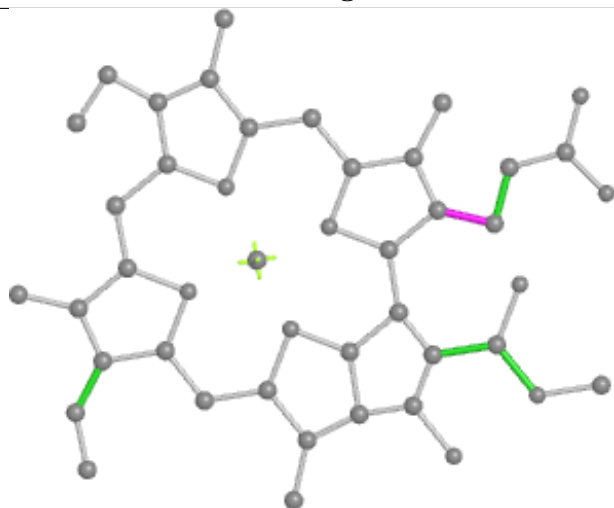
Ligand CLA B1 834



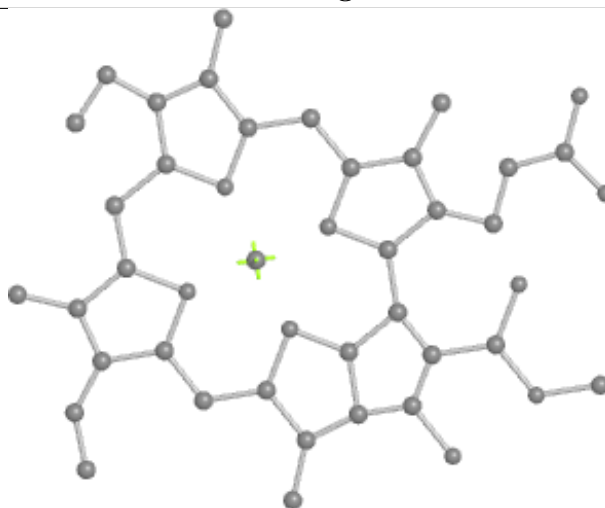
Bond lengths



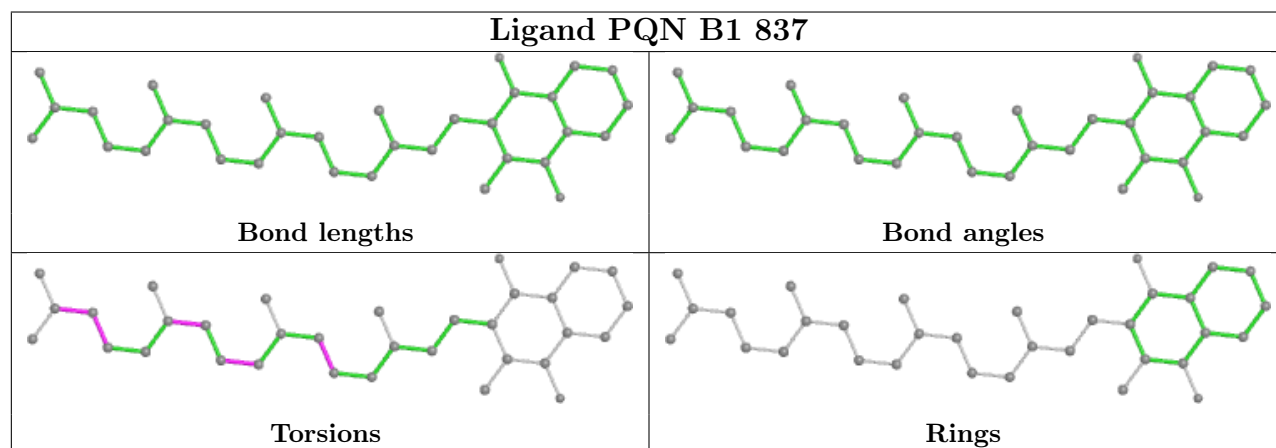
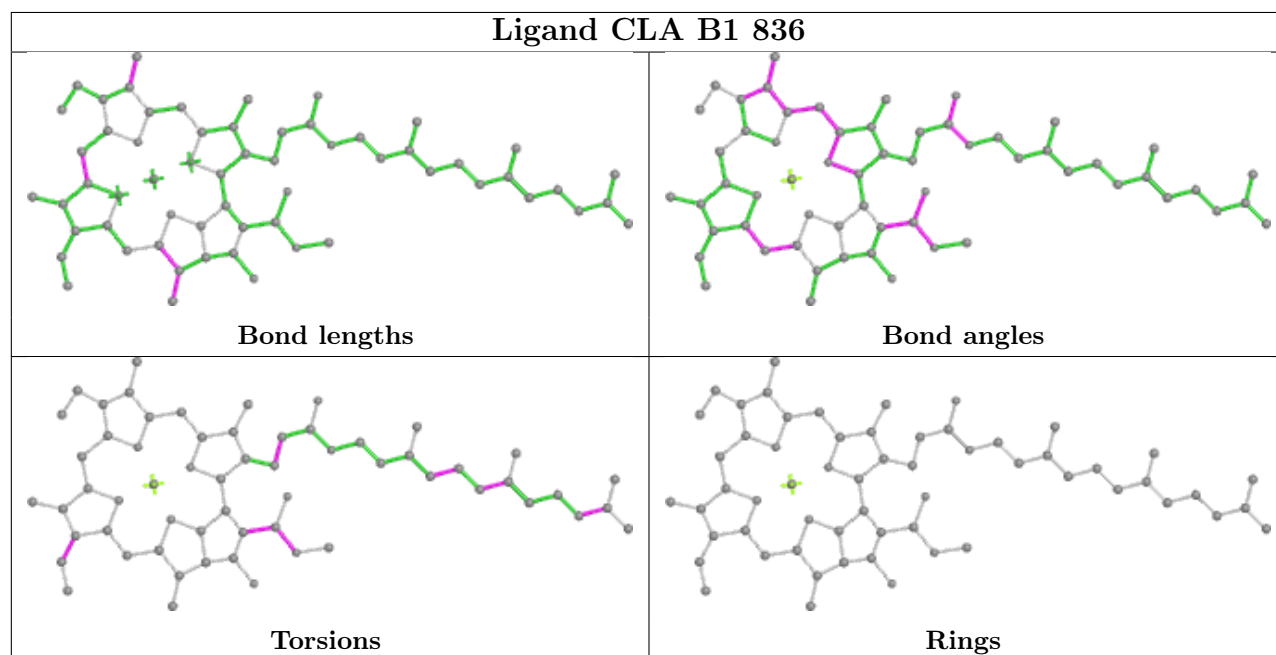
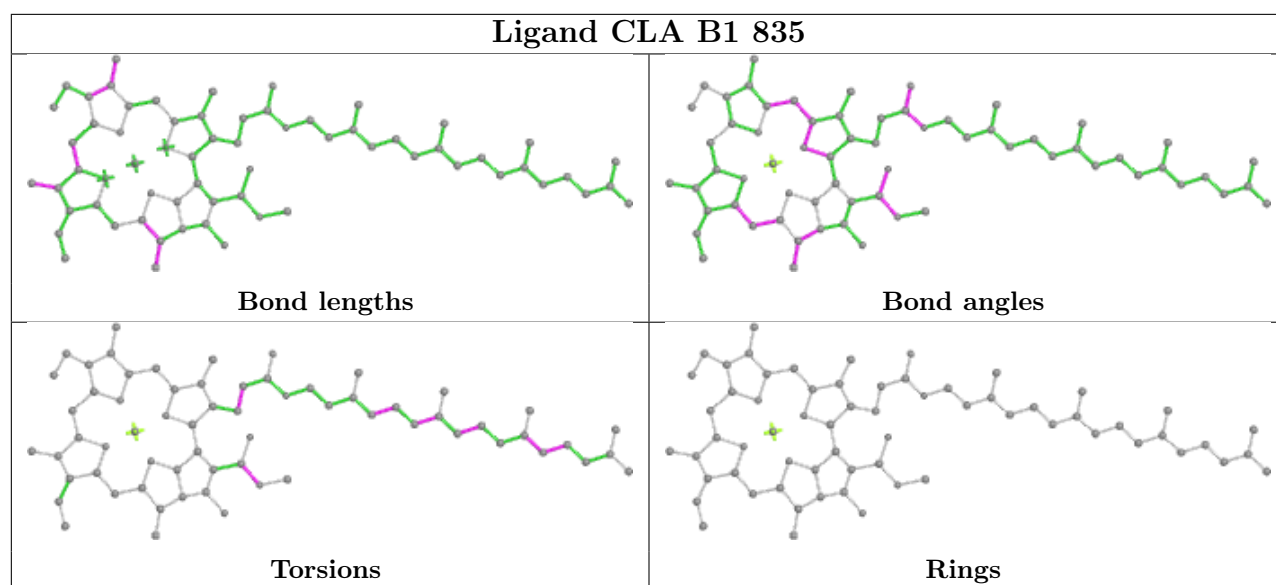
Bond angles

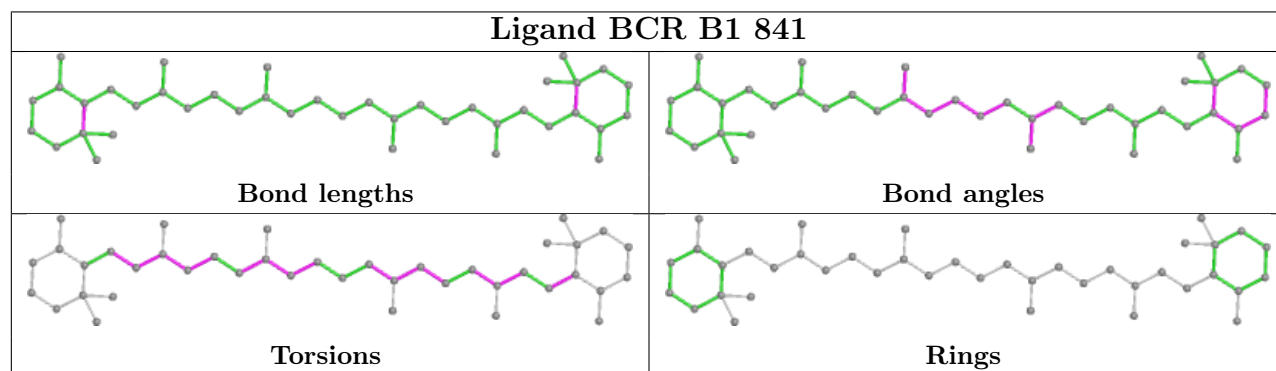
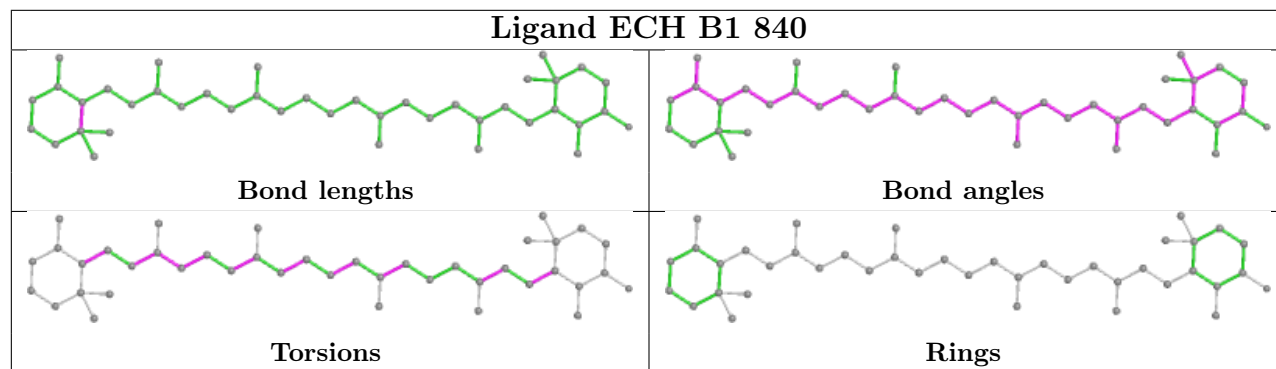
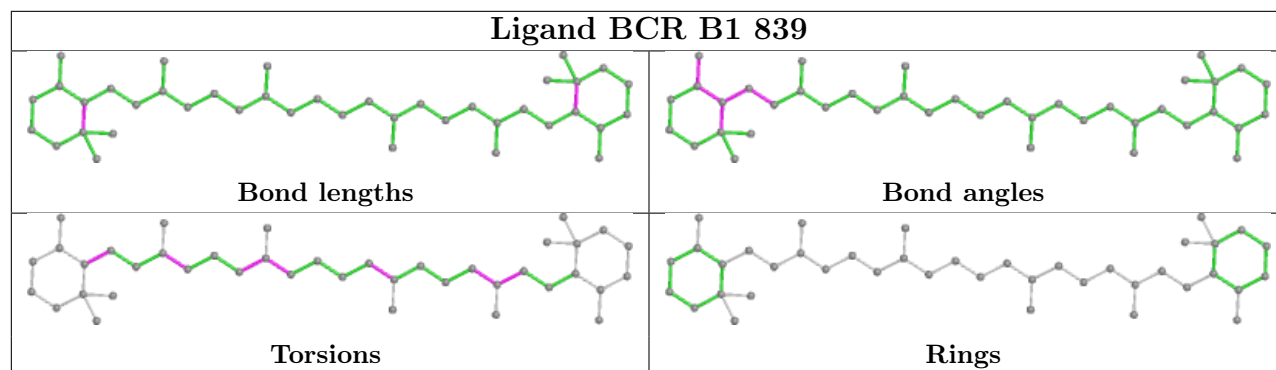
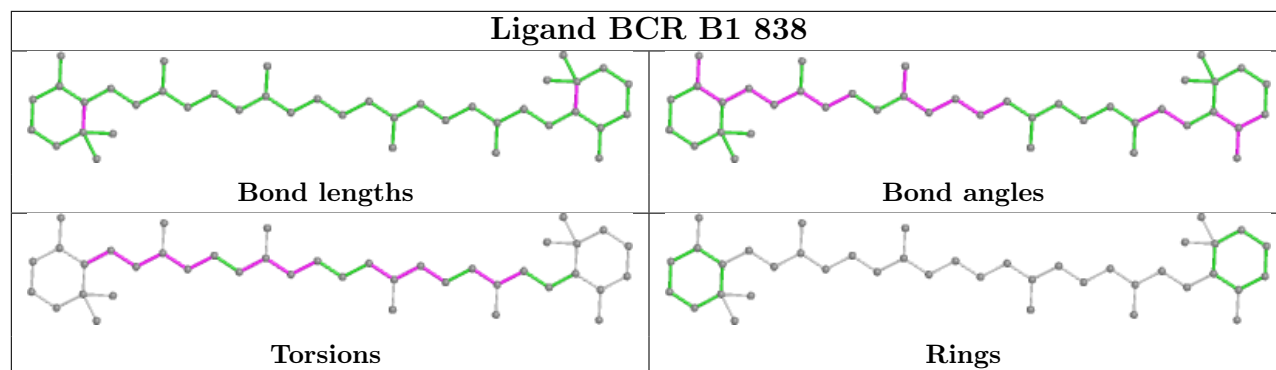


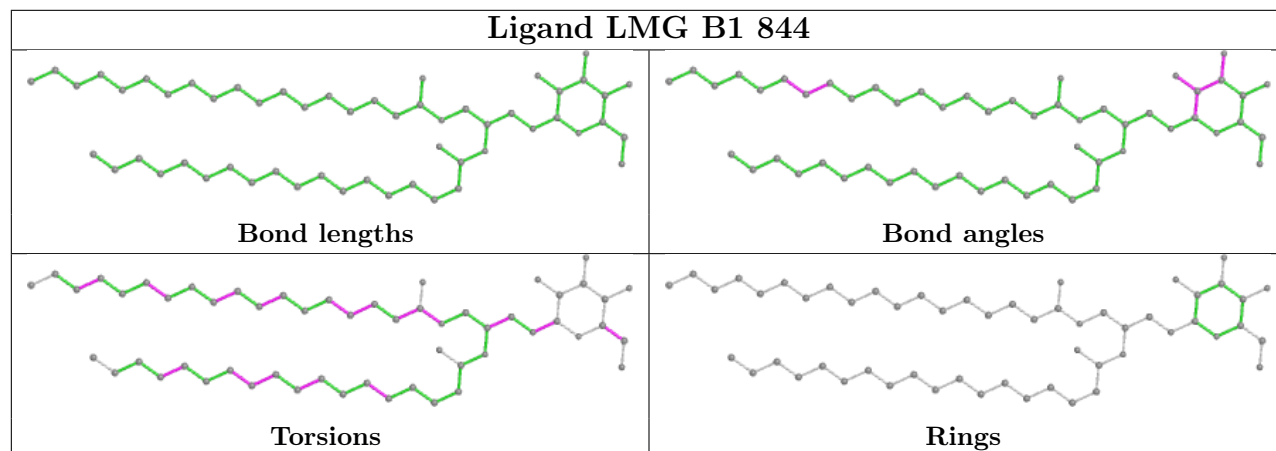
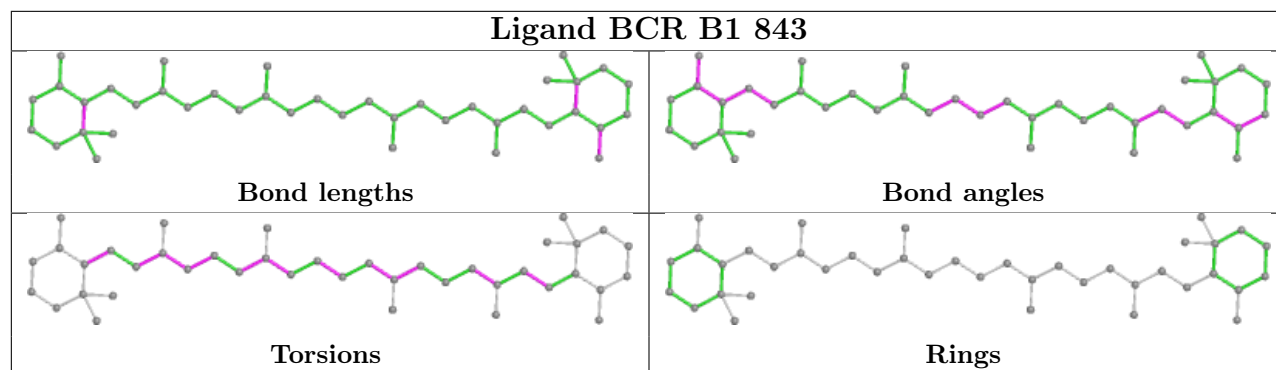
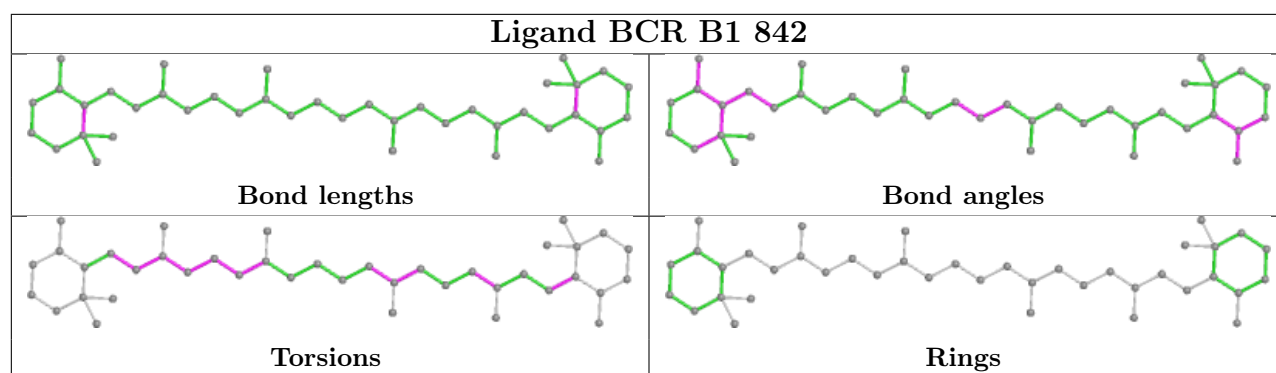
Torsions



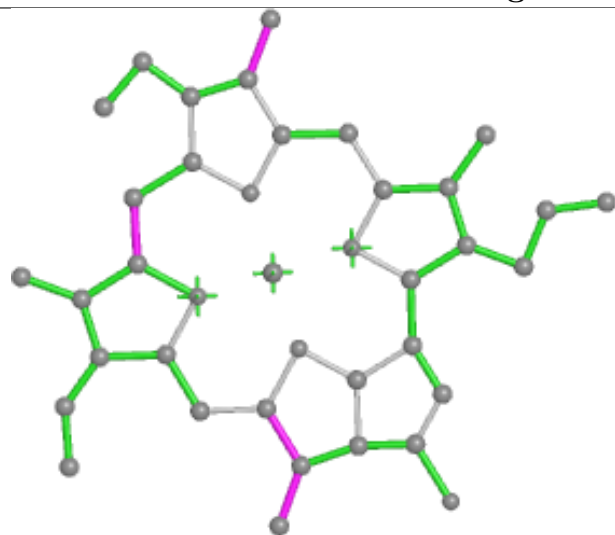
Rings



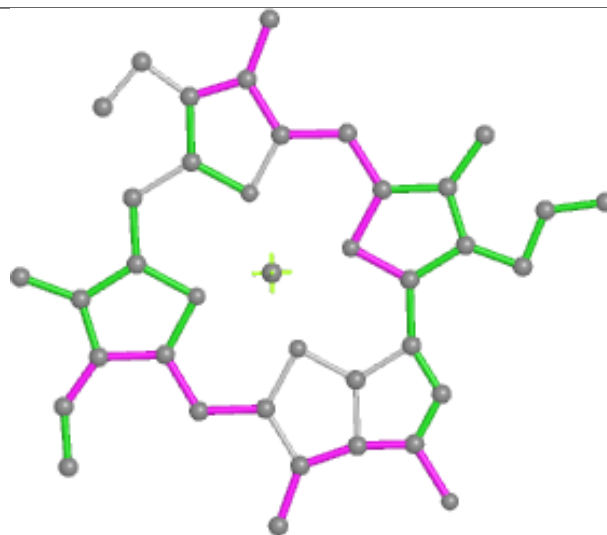




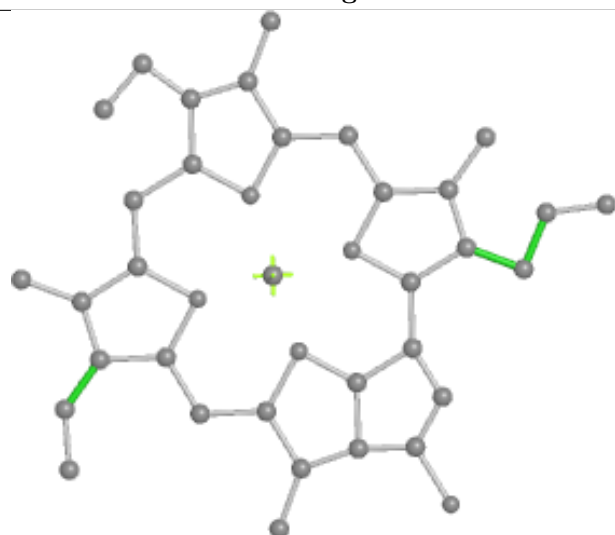
Ligand CLA B1 845



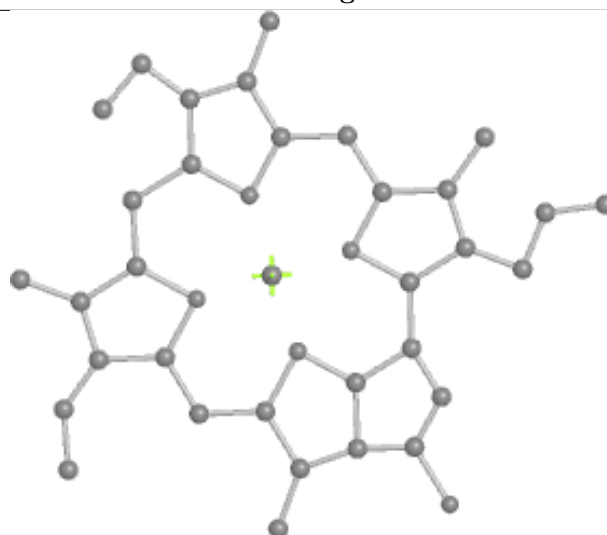
Bond lengths



Bond angles

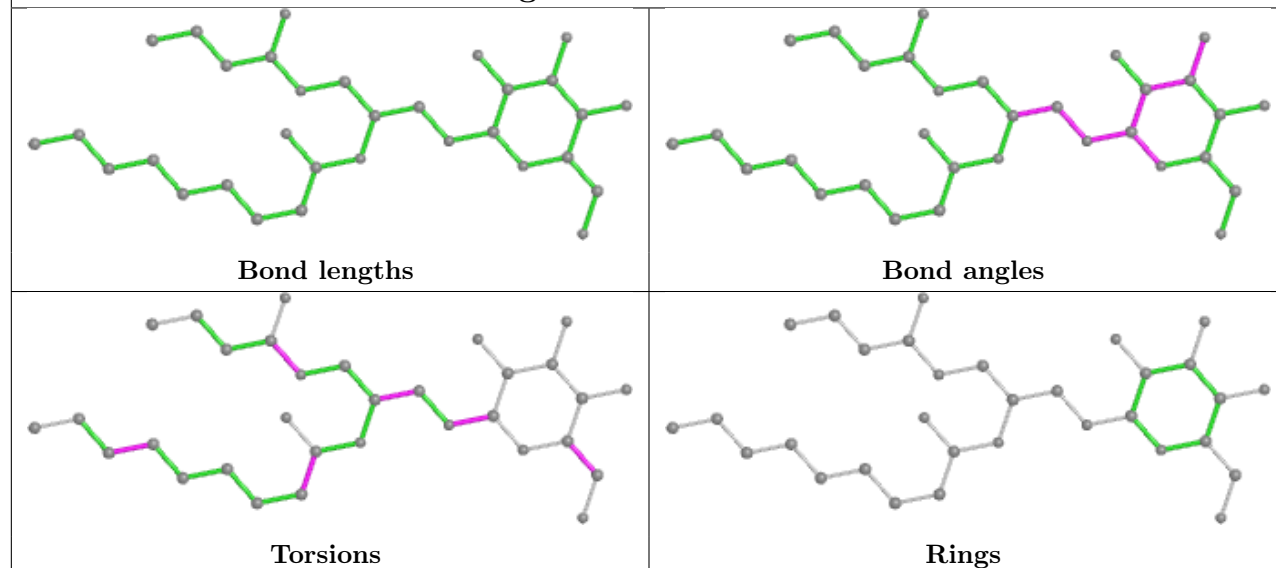


Torsions

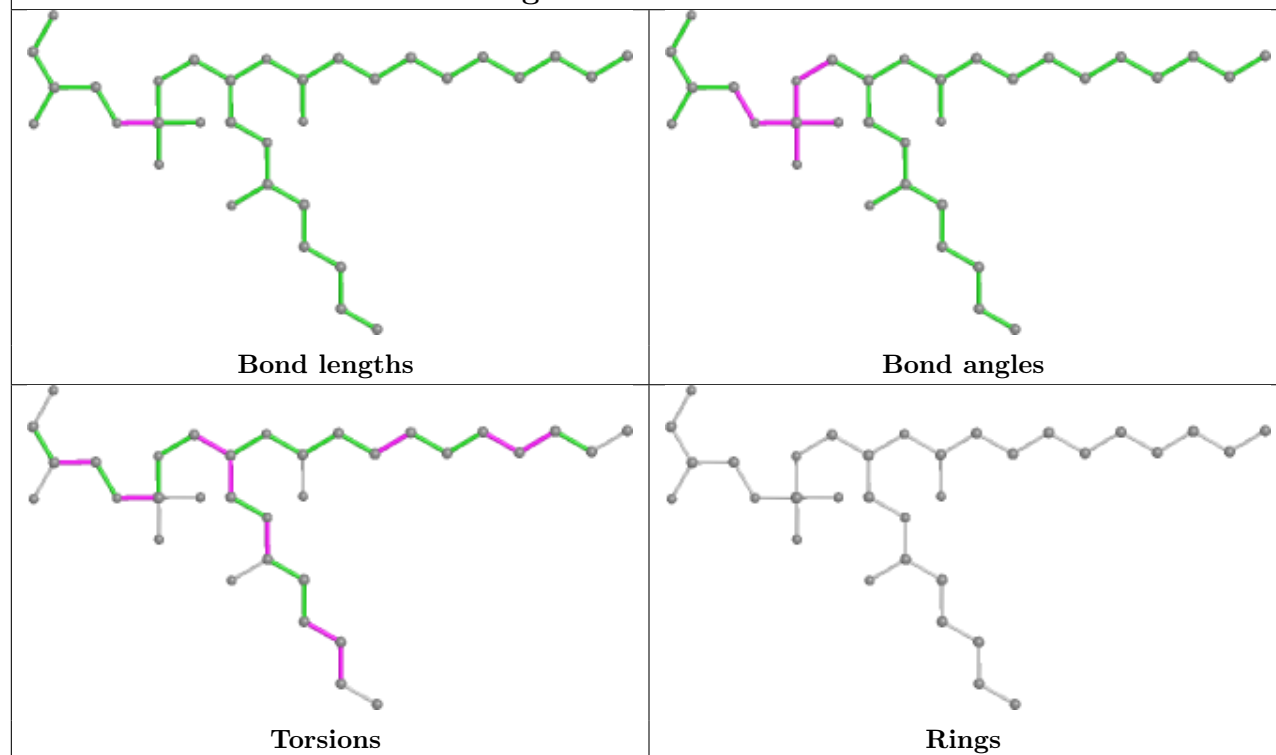


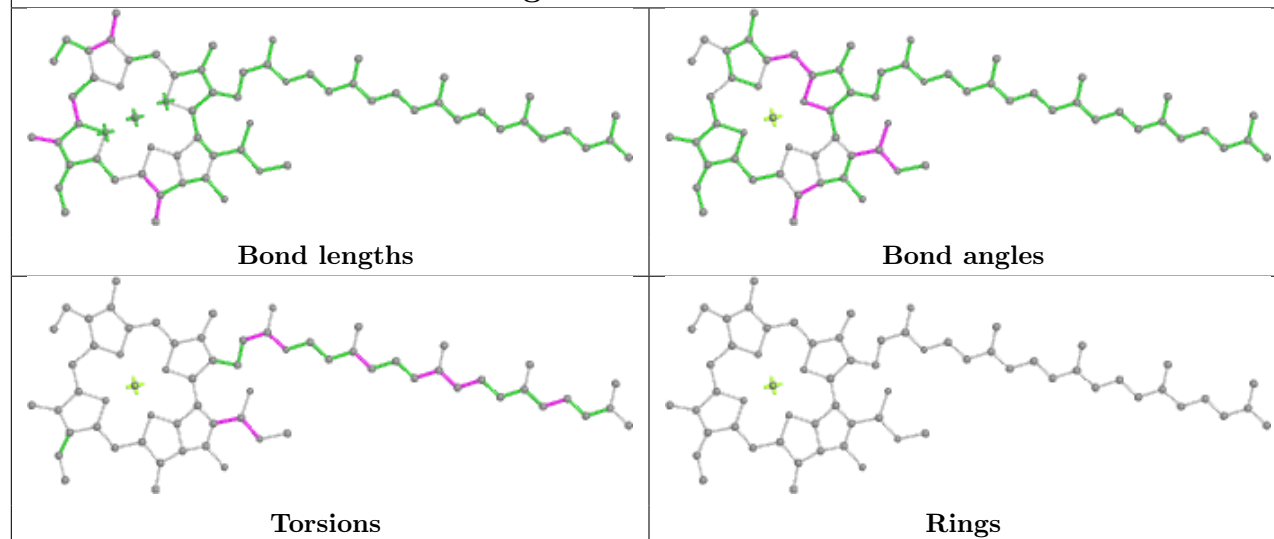
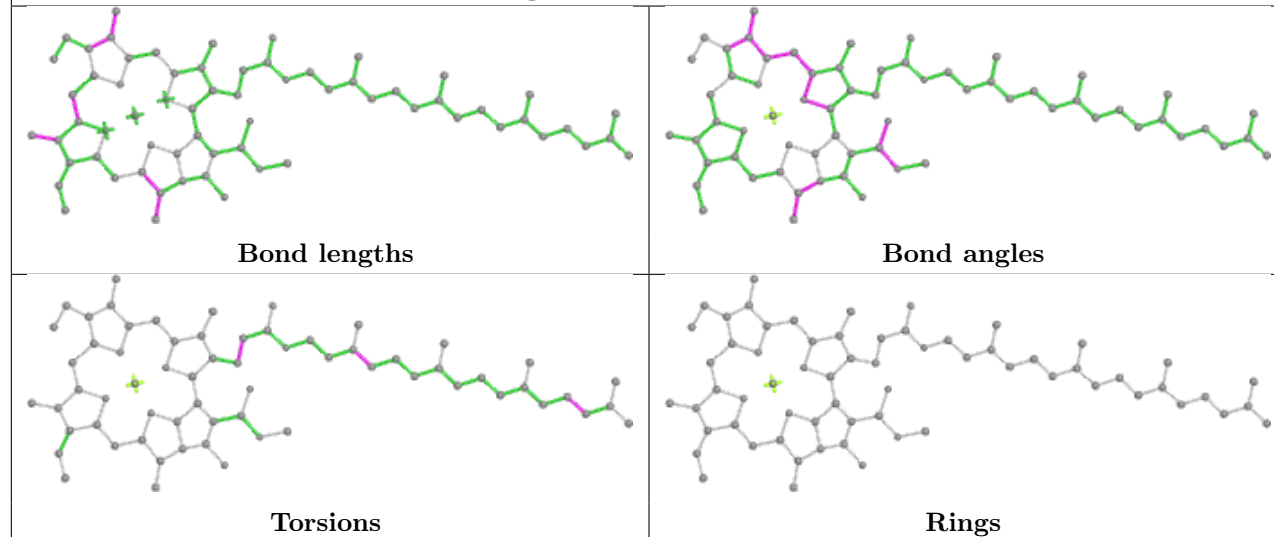
Rings

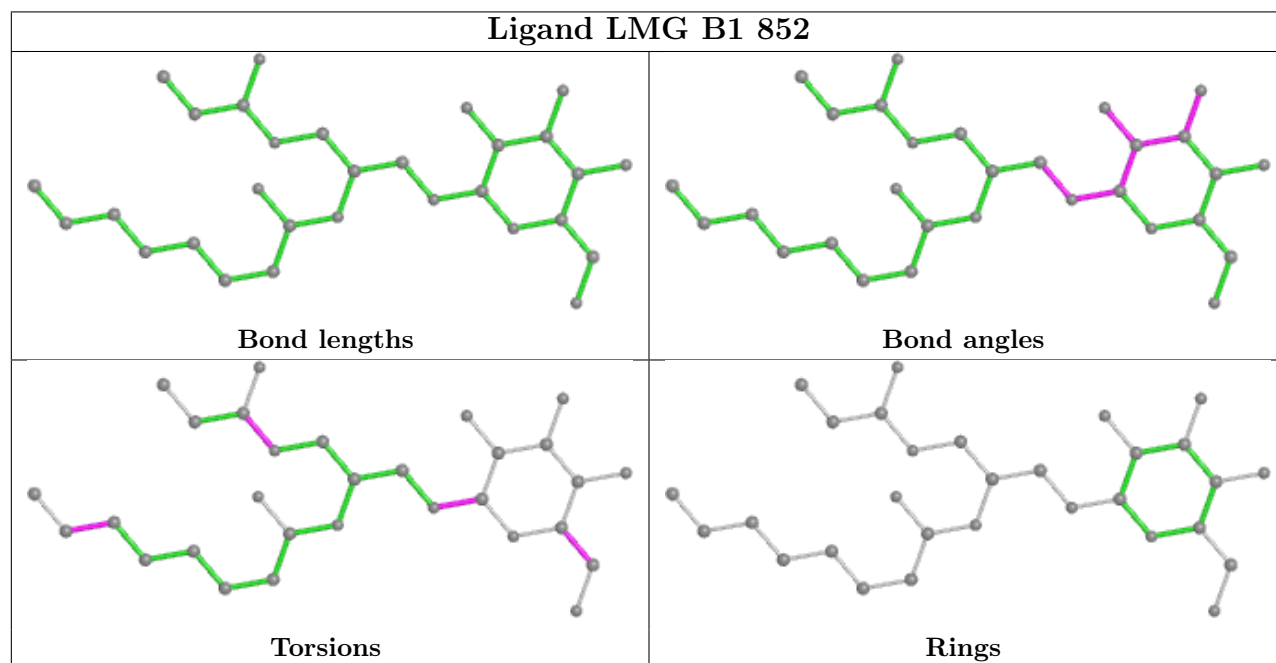
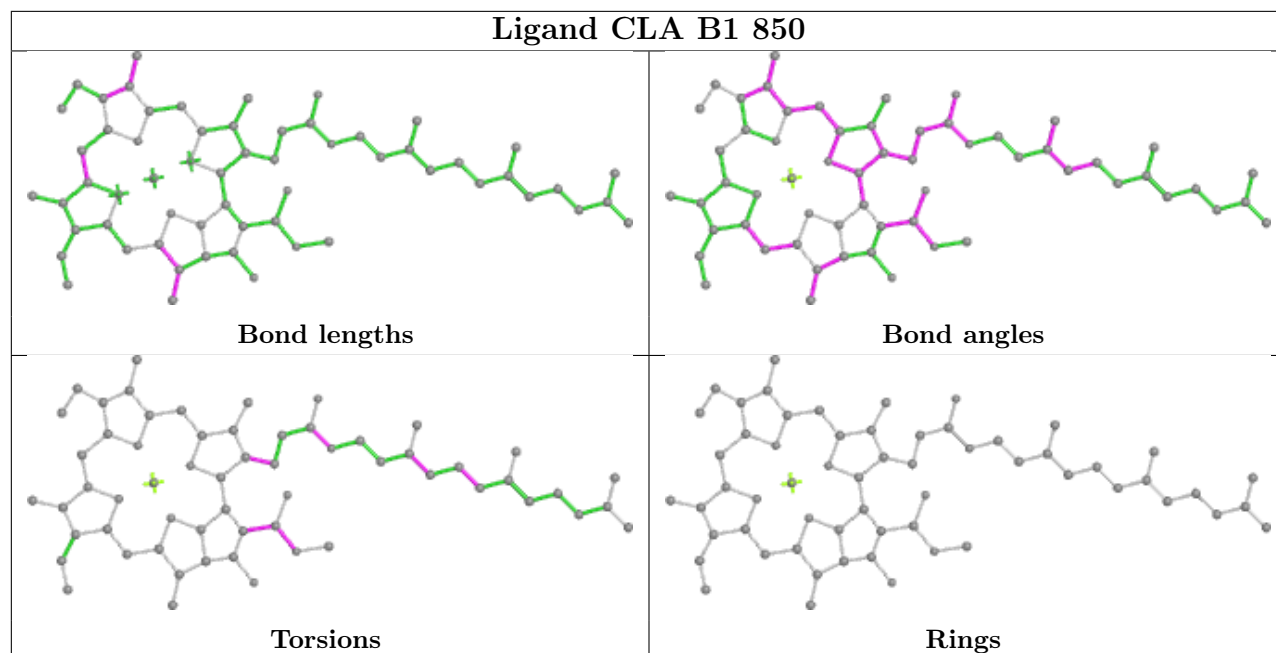
Ligand LMG B1 846

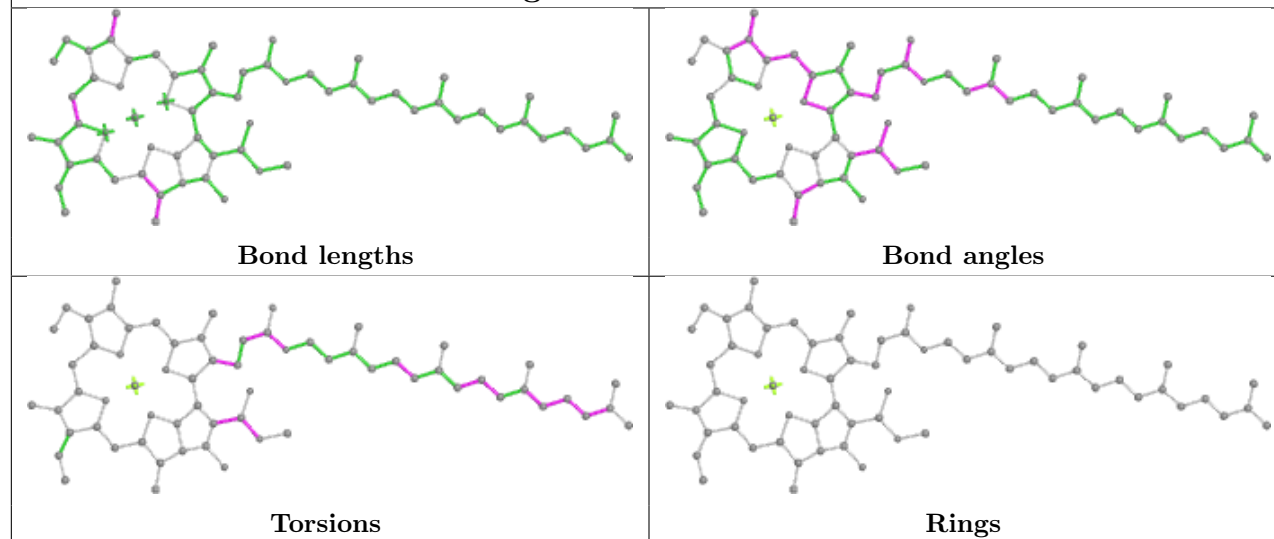
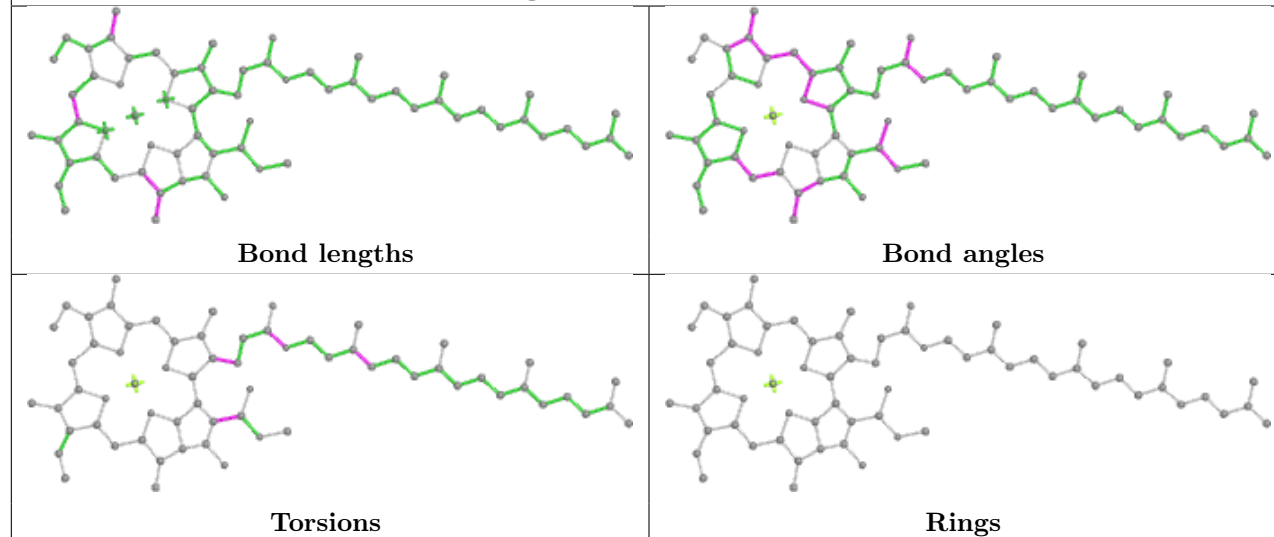
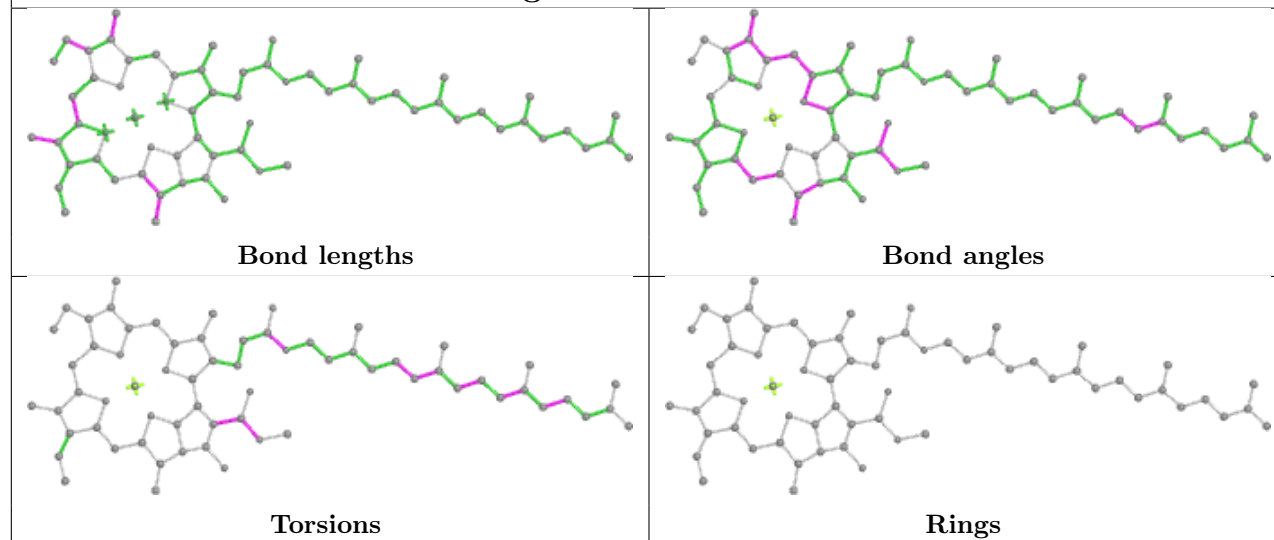


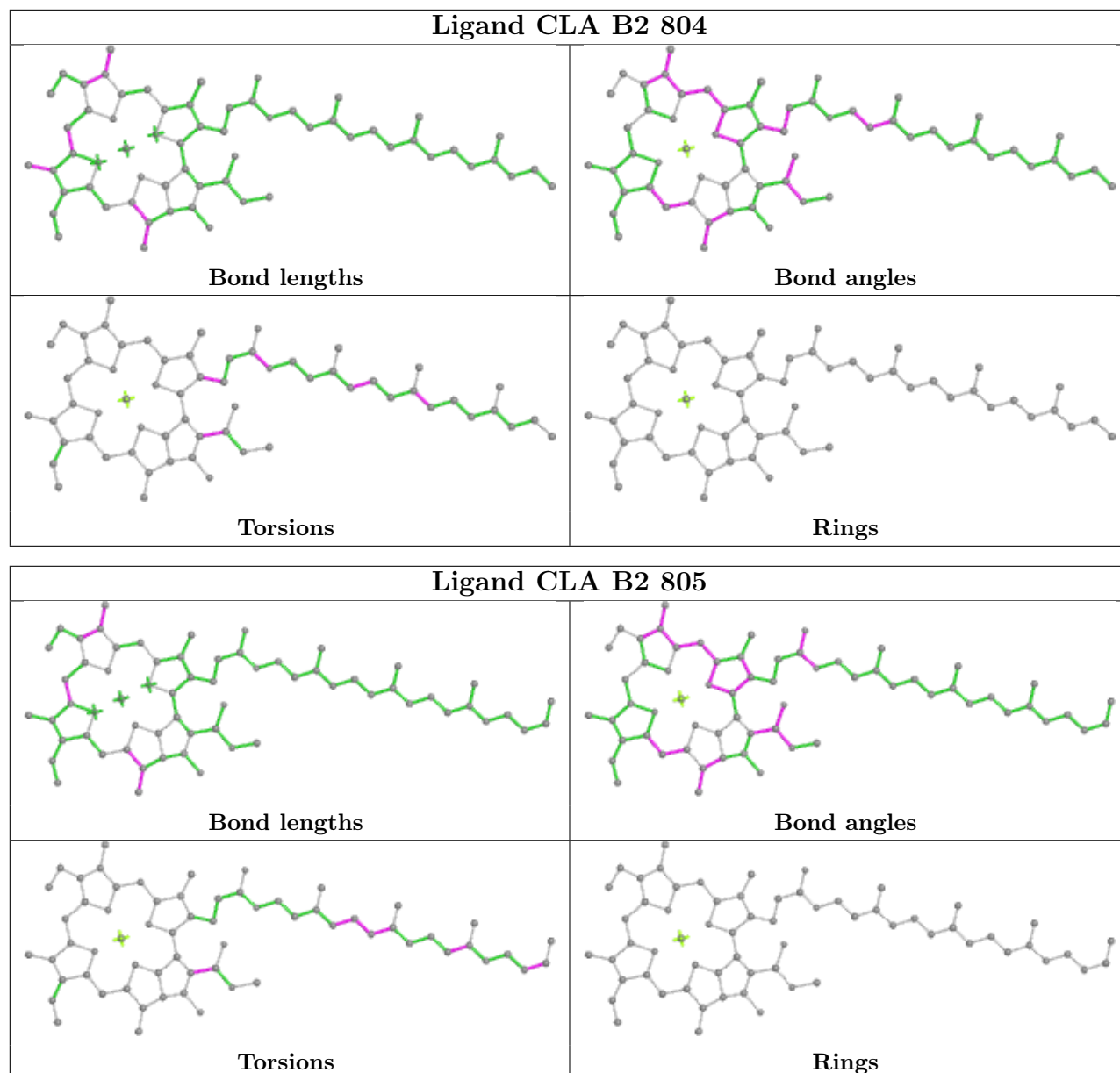
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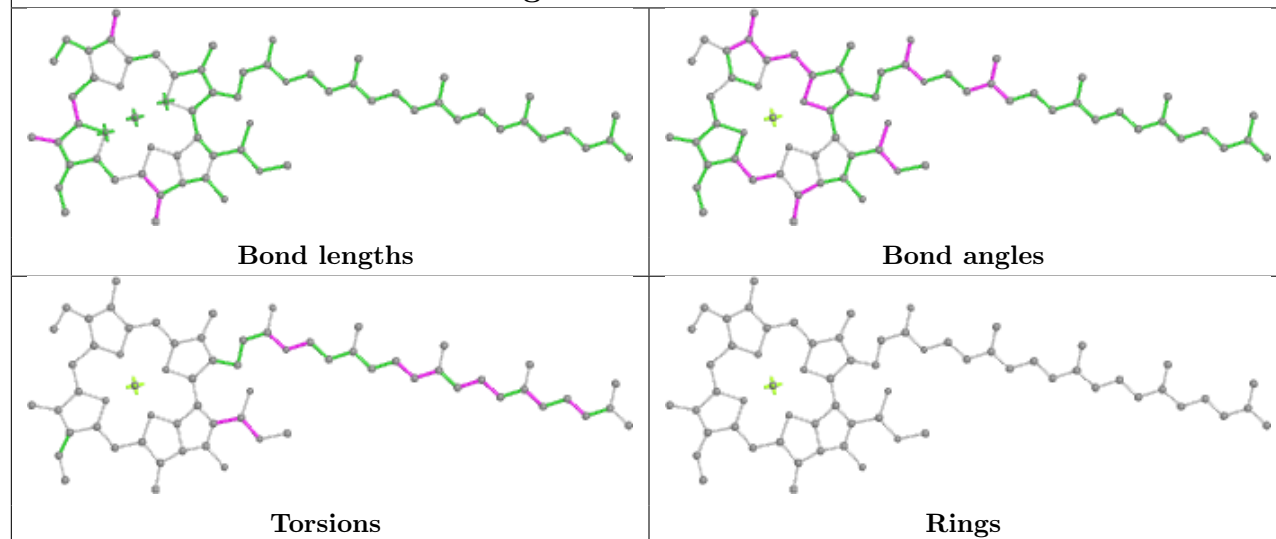
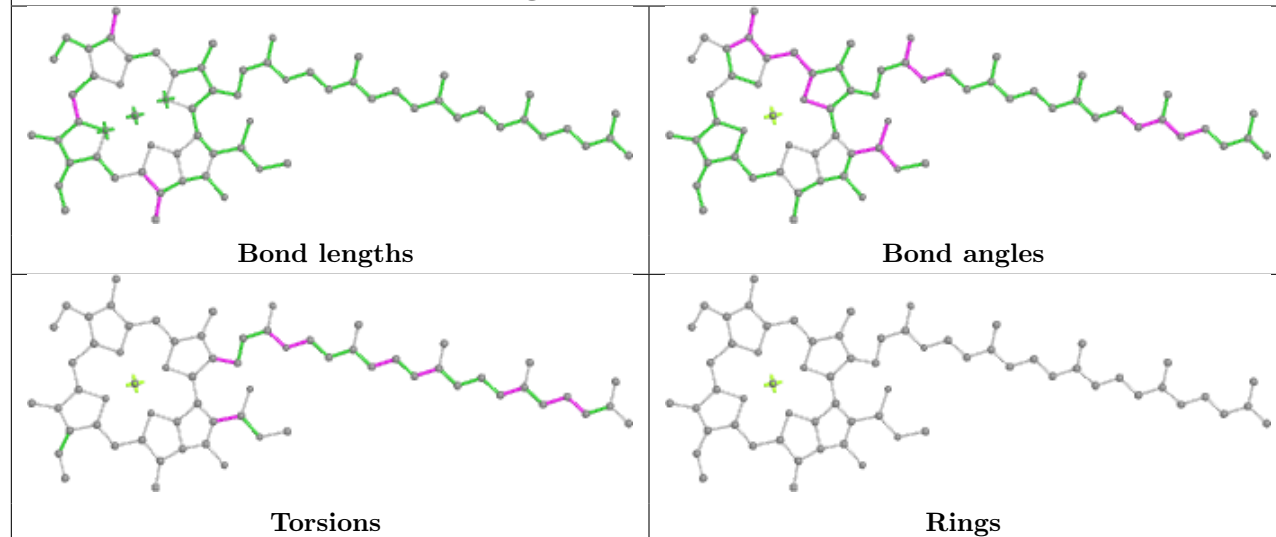


Ligand CLA B1 848**Ligand CLA B1 849**

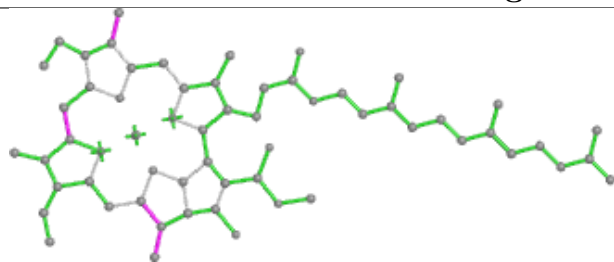


Ligand CLA B2 801**Ligand CLA B2 802****Ligand CLA B2 803**

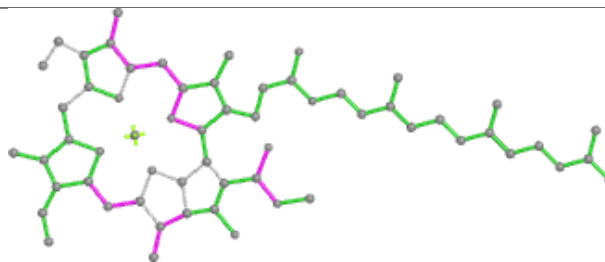


Ligand CLA B2 806**Ligand CLA B2 807**

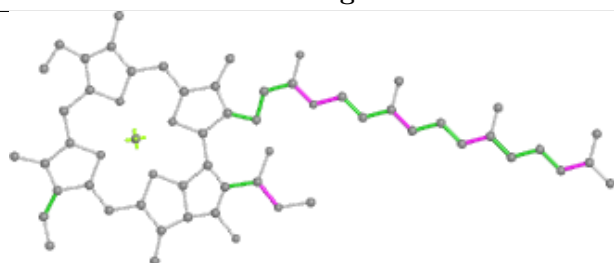
Ligand CLA B2 808



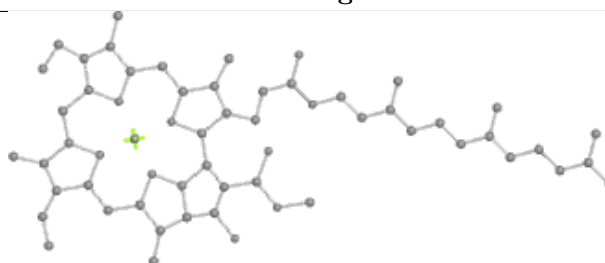
Bond lengths



Bond angles

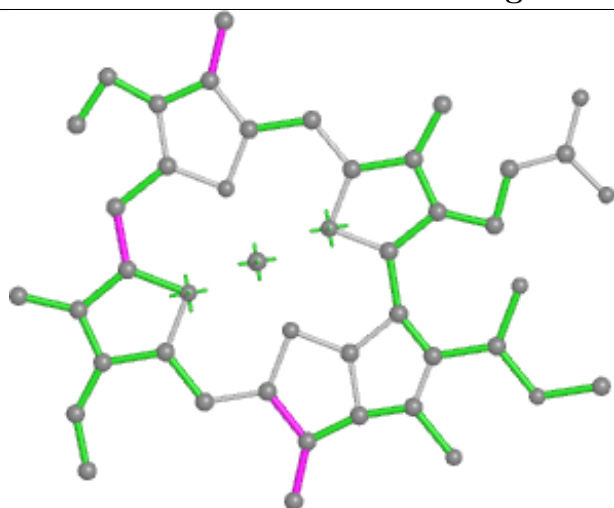


Torsions

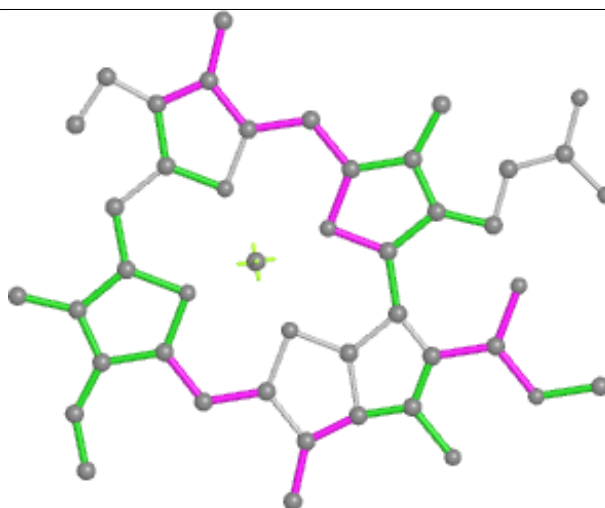


Rings

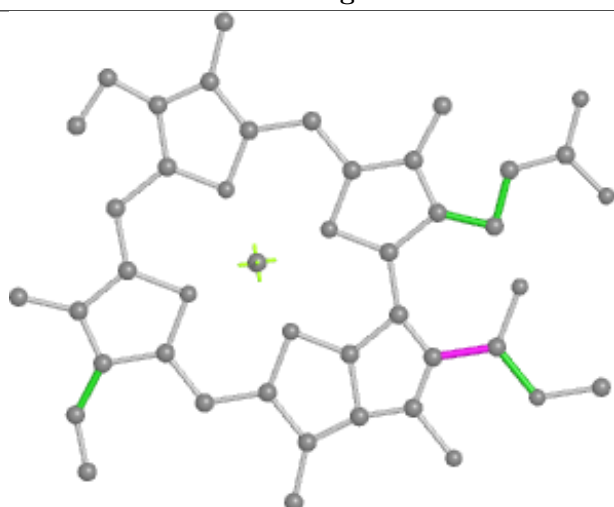
Ligand CLA B2 809



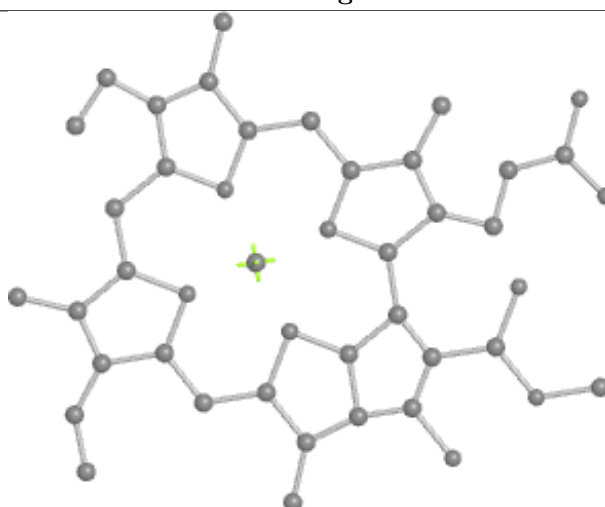
Bond lengths



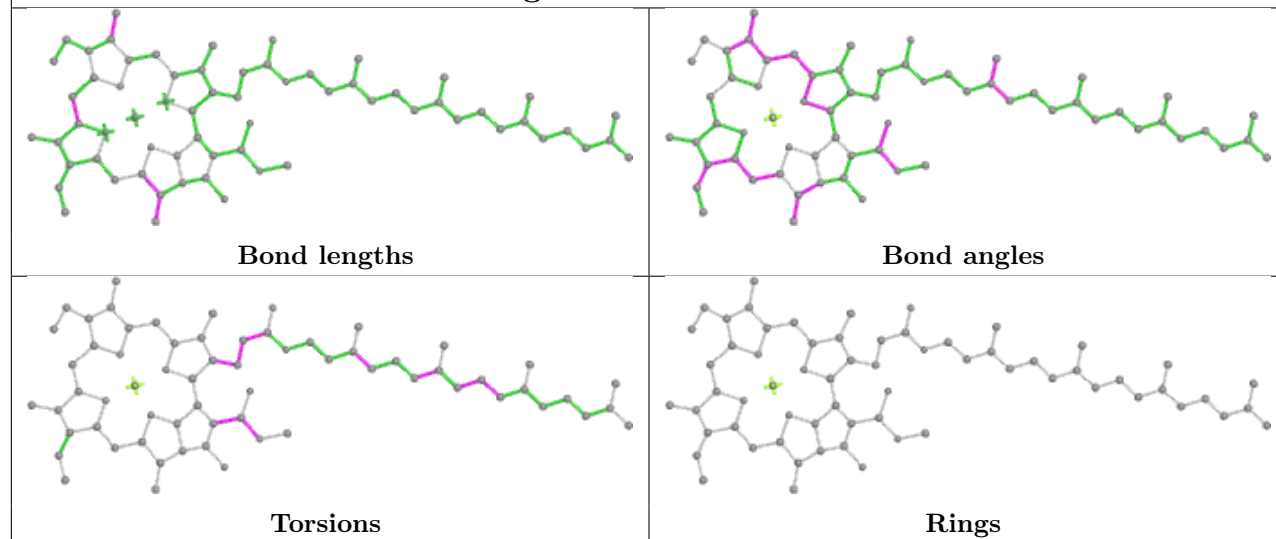
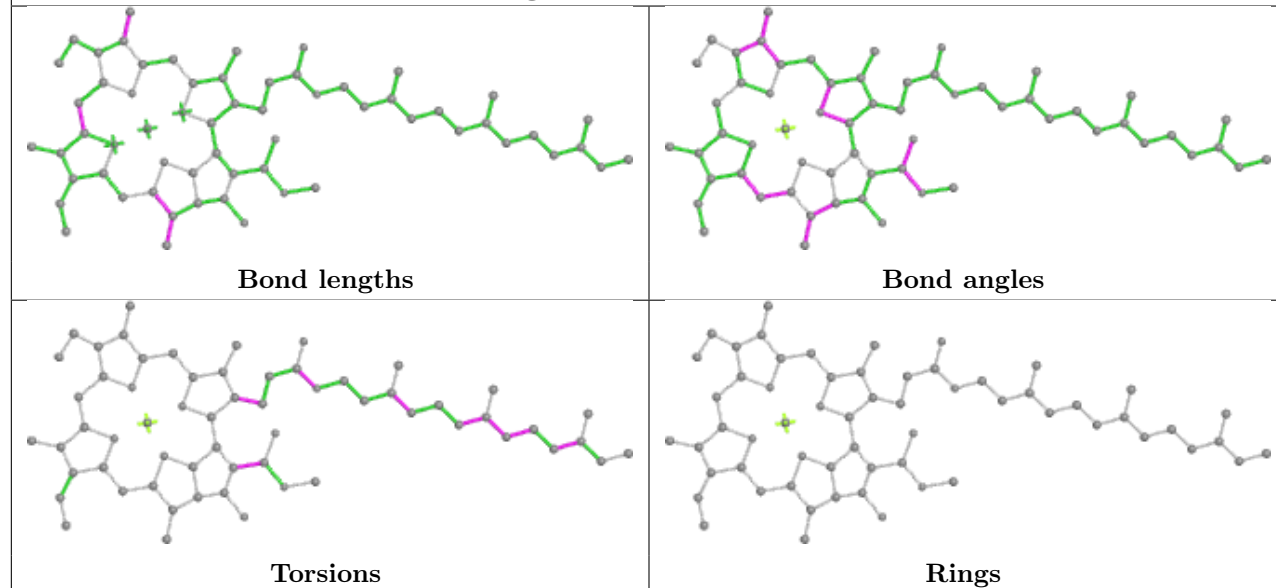
Bond angles



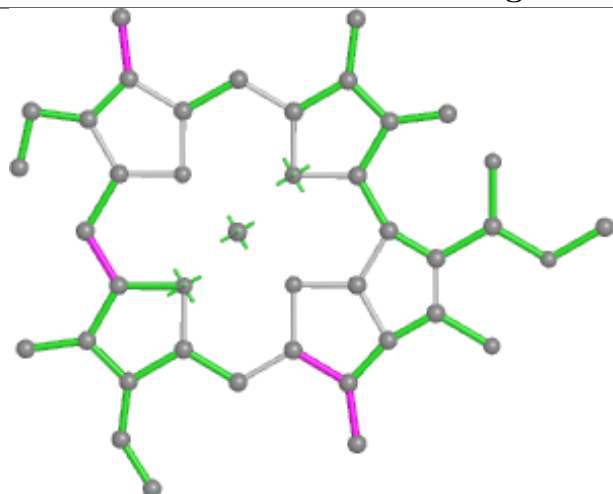
Torsions



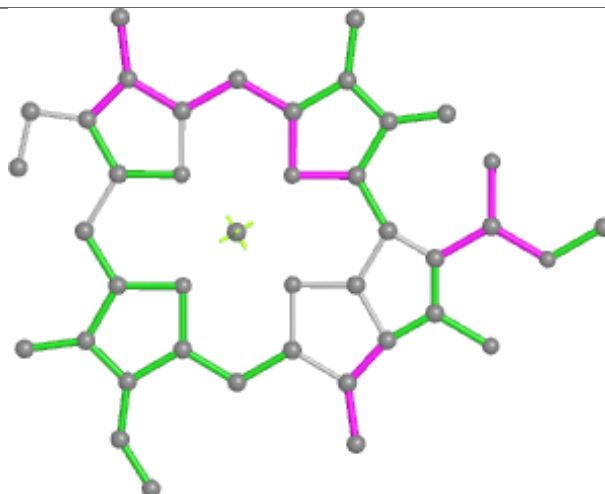
Rings

Ligand CLA B2 810**Ligand CLA B2 811**

Ligand CLA B2 812



Bond lengths



Bond angles

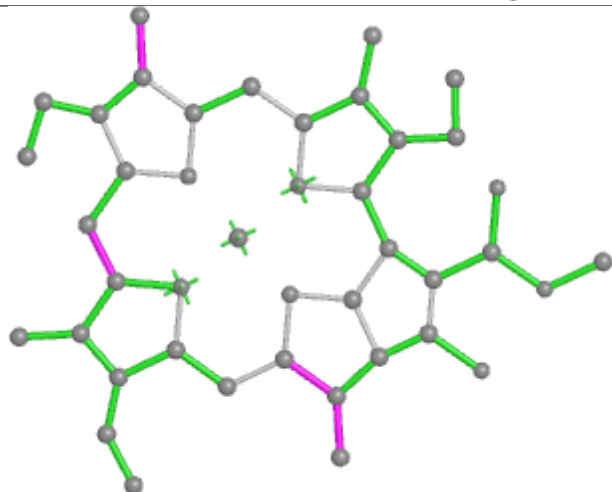


Torsions

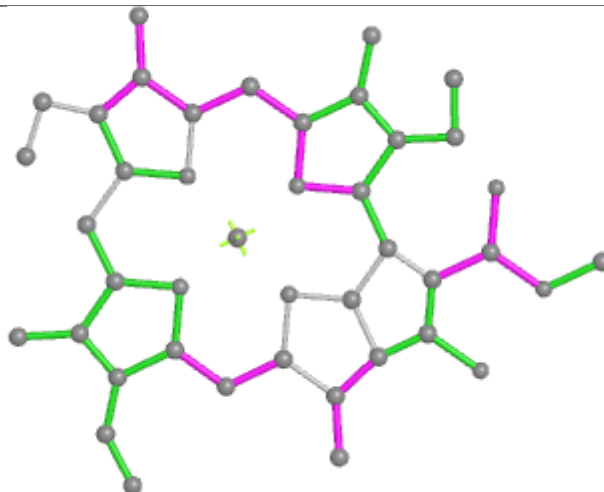


Rings

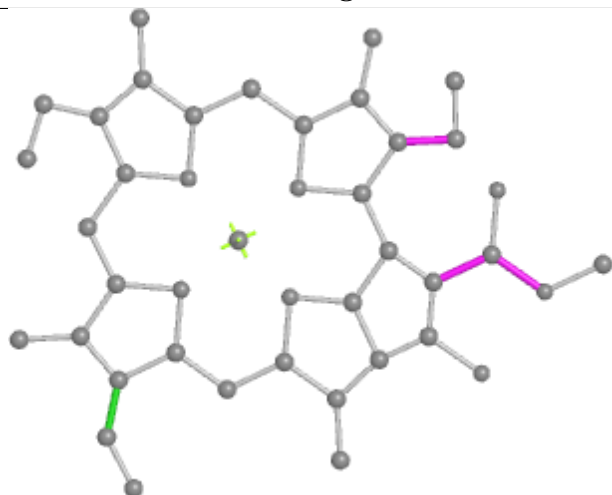
Ligand CLA B2 813



Bond lengths



Bond angles

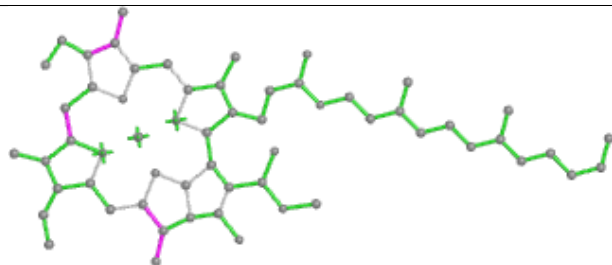


Torsions

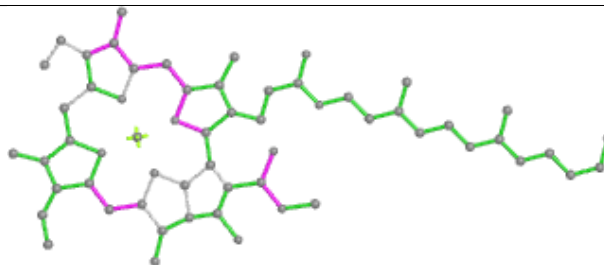


Rings

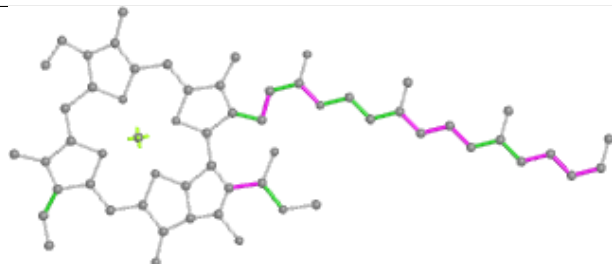
Ligand CLA B2 814



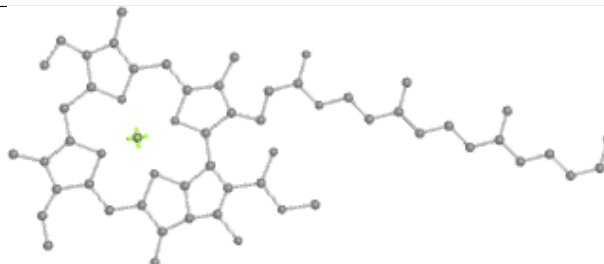
Bond lengths



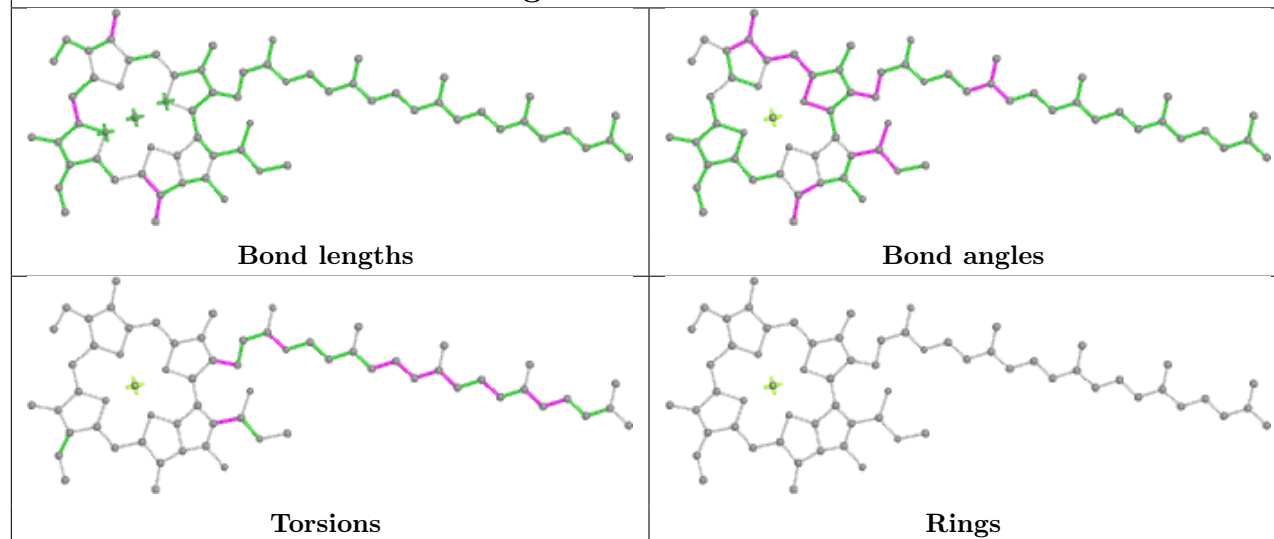
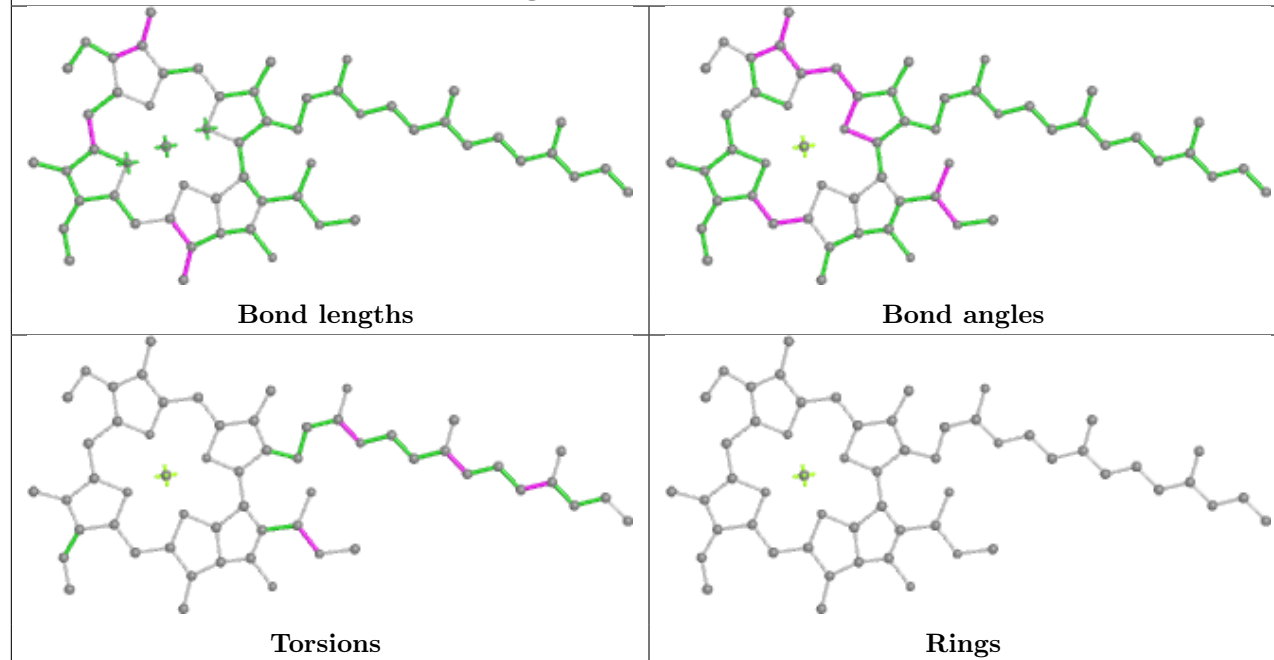
Bond angles



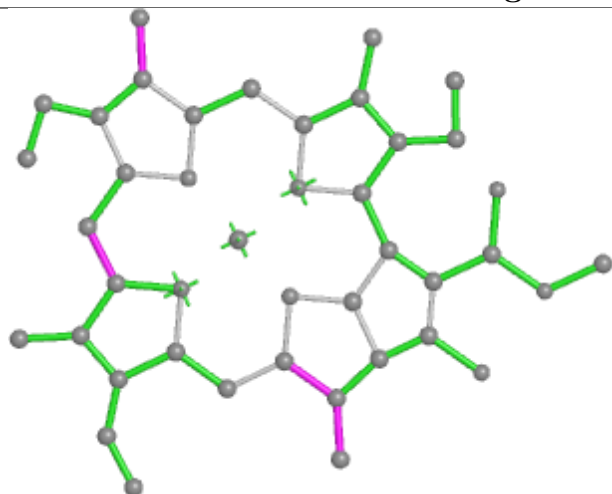
Torsions



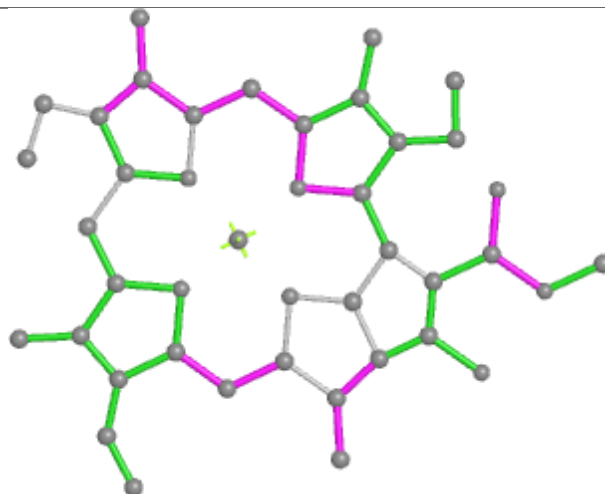
Rings

Ligand CLA B2 815**Ligand CLA B2 816**

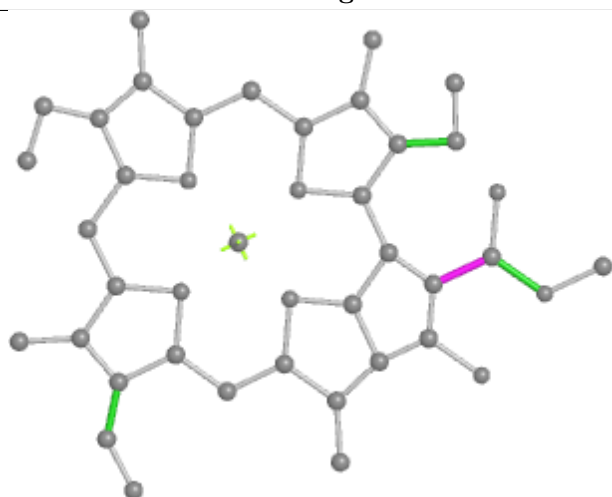
Ligand CLA B2 817



Bond lengths



Bond angles

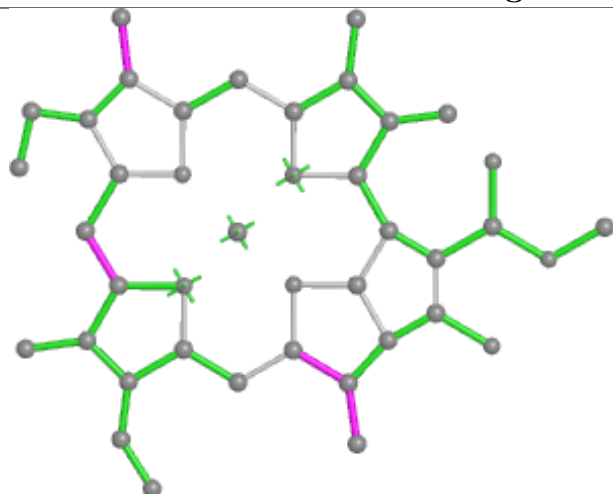


Torsions

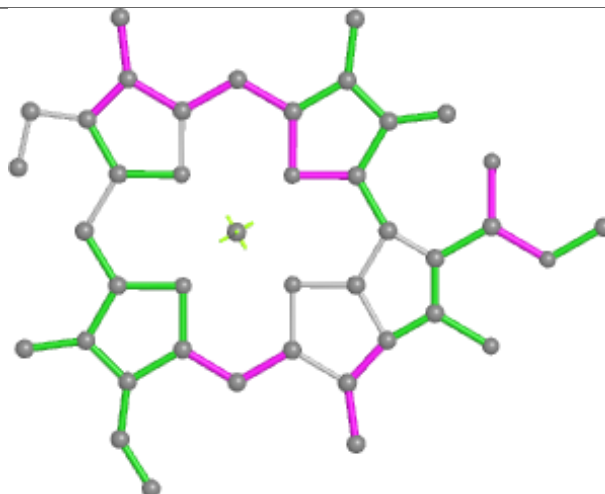


Rings

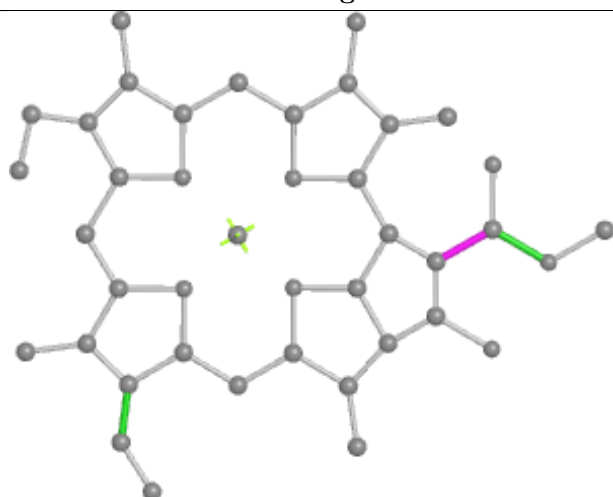
Ligand CLA B2 818



Bond lengths



Bond angles

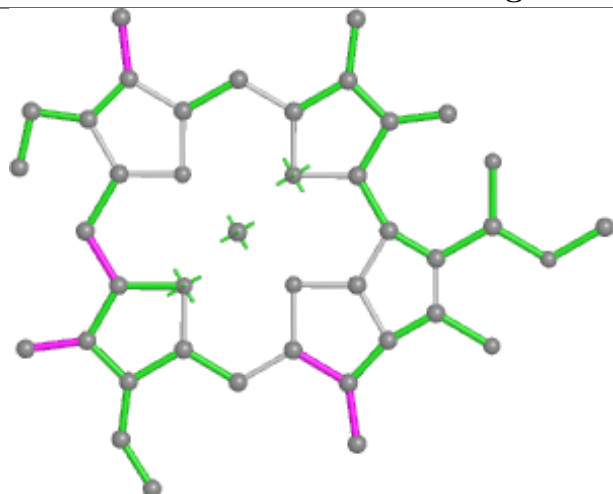


Torsions

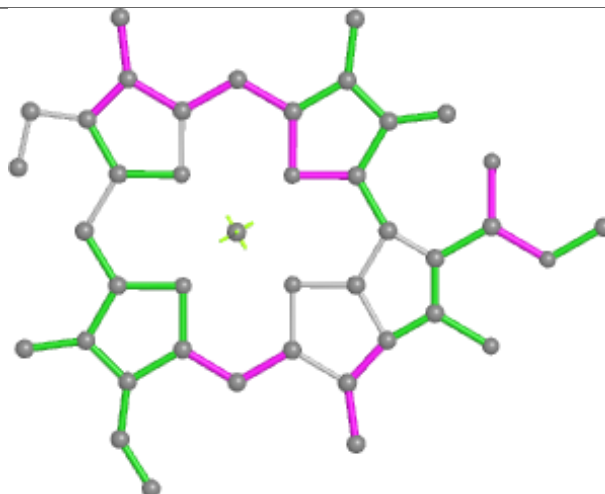


Rings

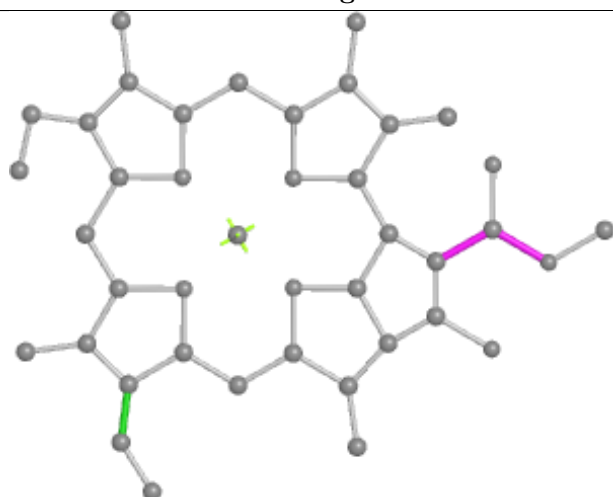
Ligand CLA B2 819



Bond lengths



Bond angles

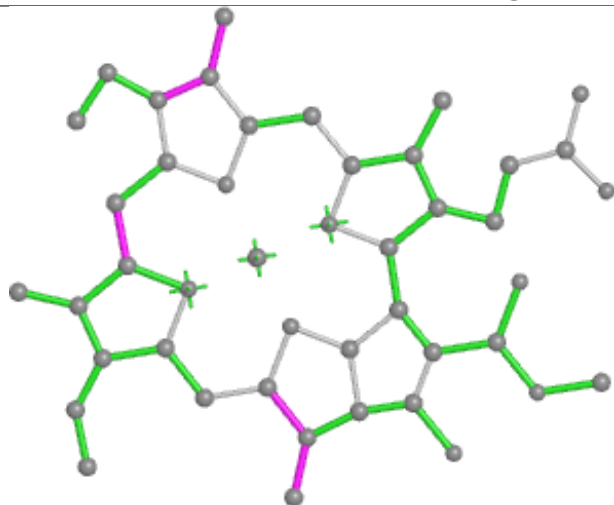


Torsions

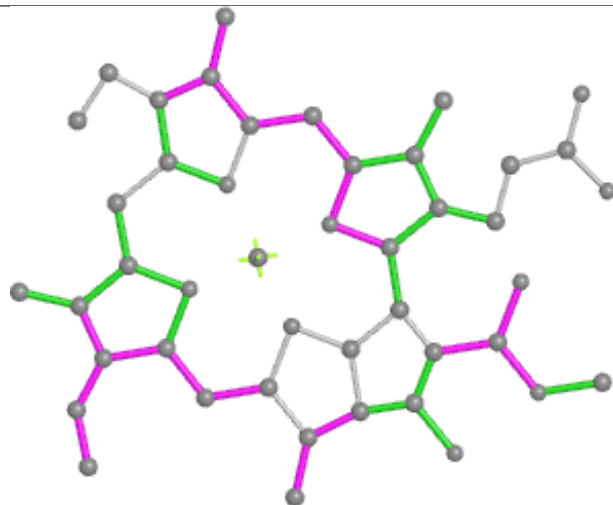


Rings

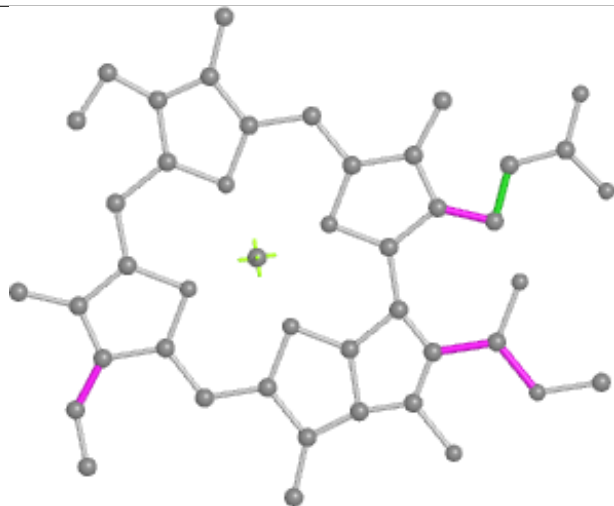
Ligand CLA B2 820



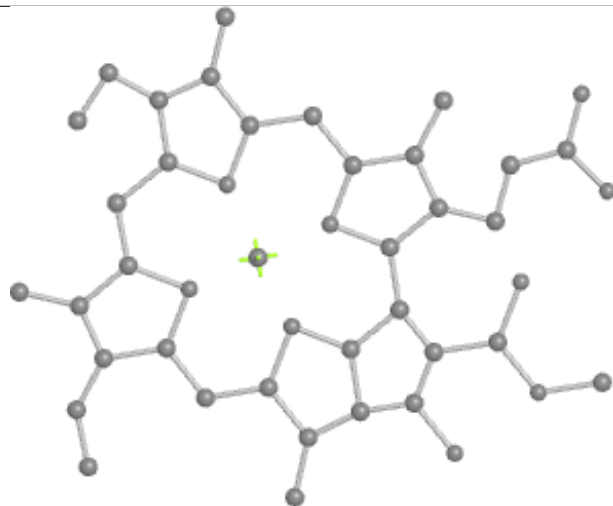
Bond lengths



Bond angles

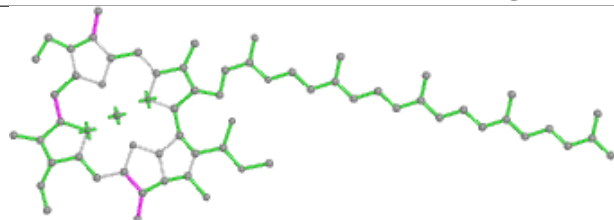


Torsions

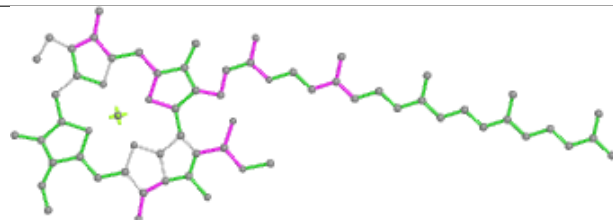


Rings

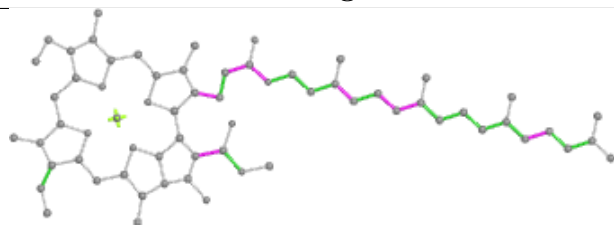
Ligand CLA B2 821



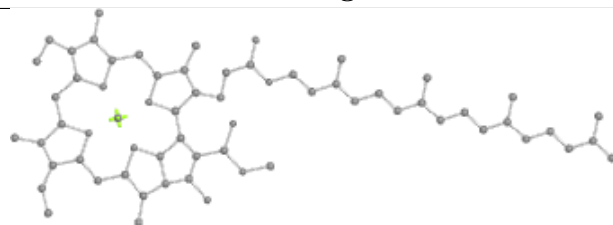
Bond lengths



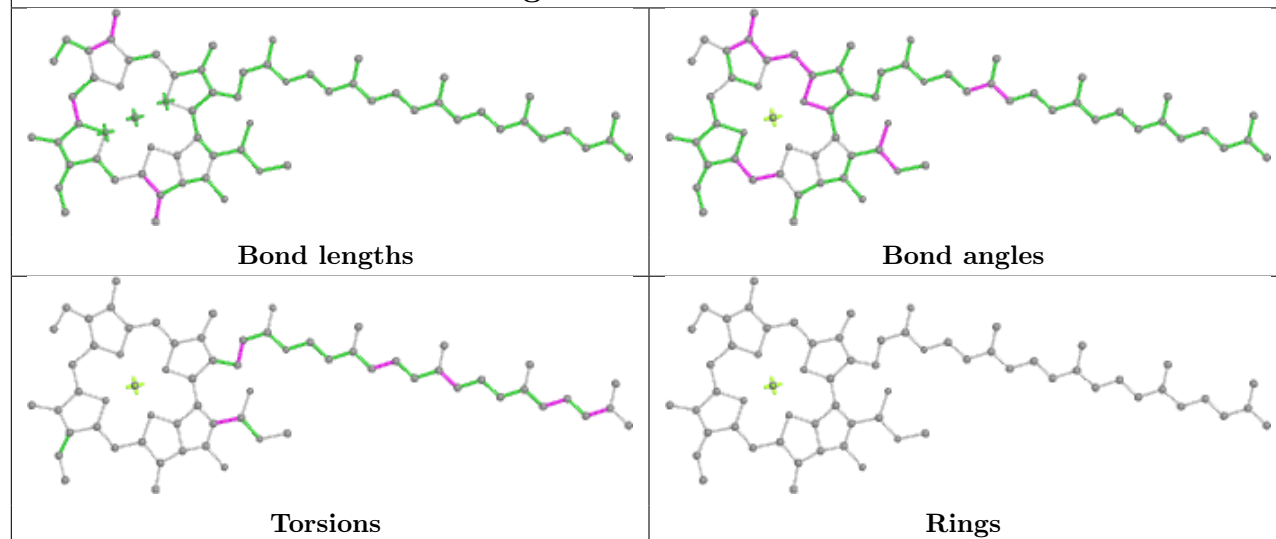
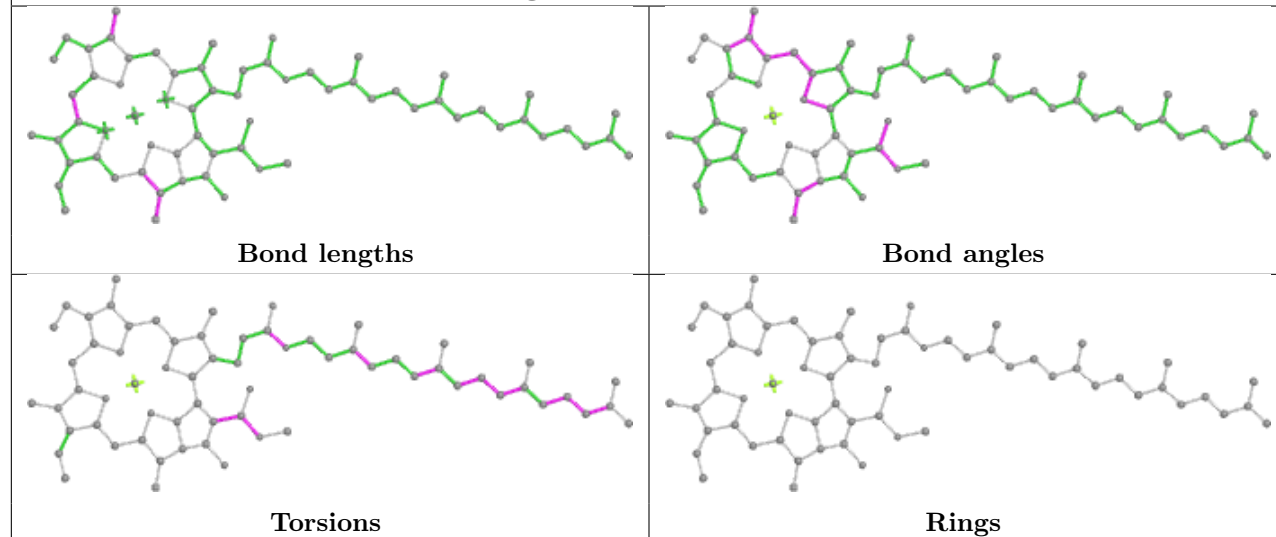
Bond angles



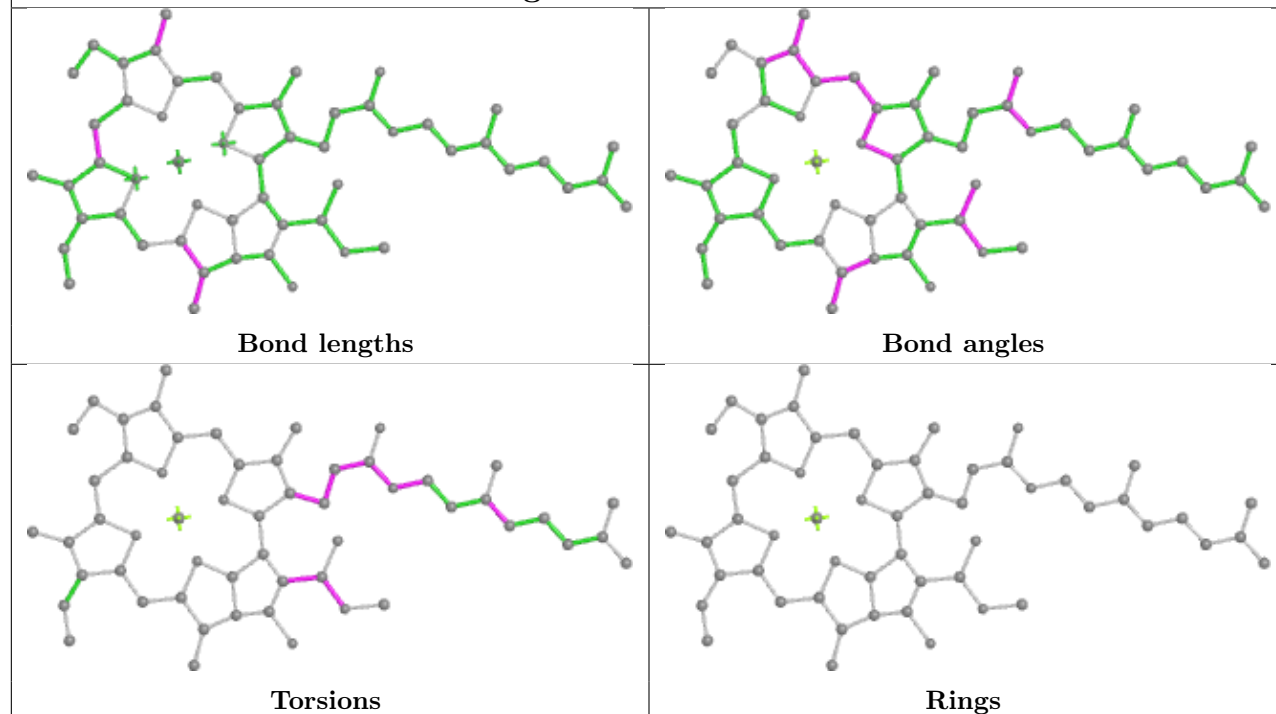
Torsions



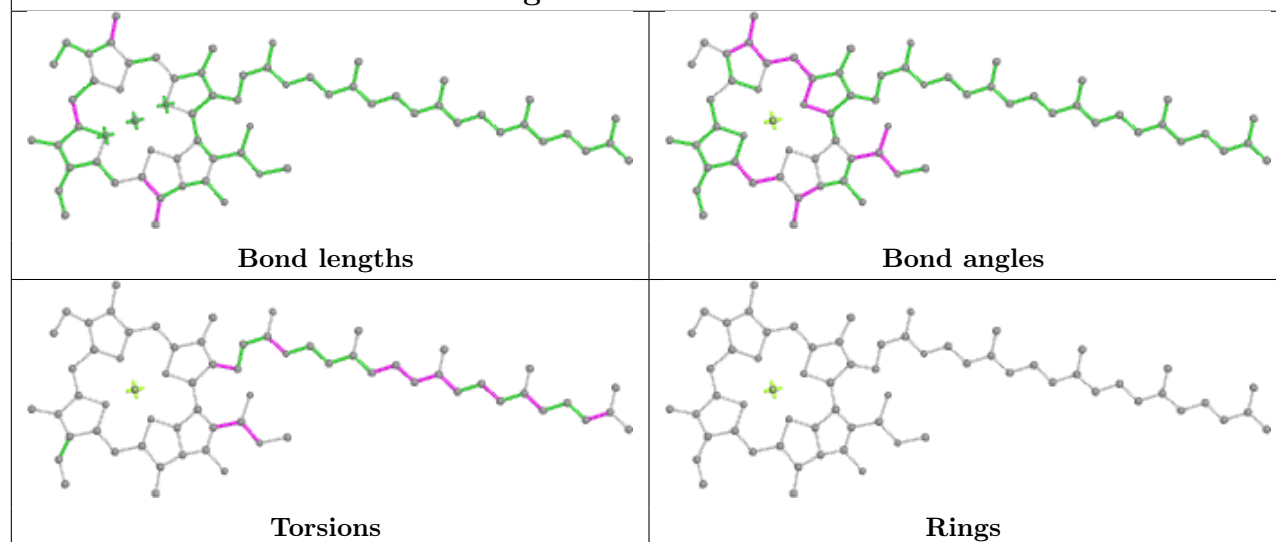
Rings

Ligand CLA B2 822**Ligand CLA B2 823**

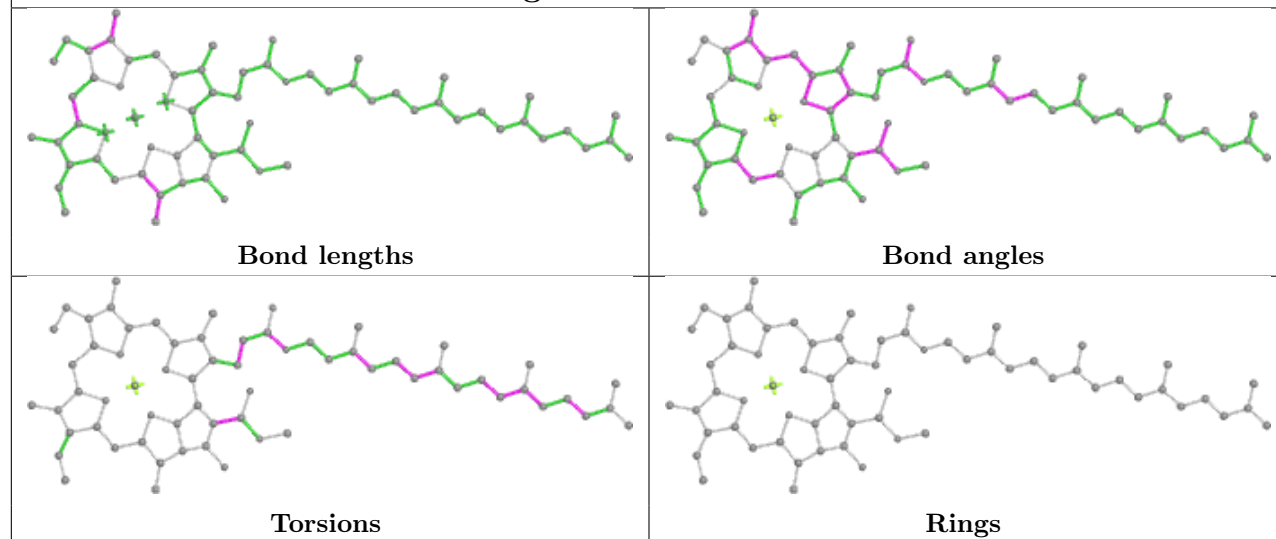
Ligand CLA B2 824



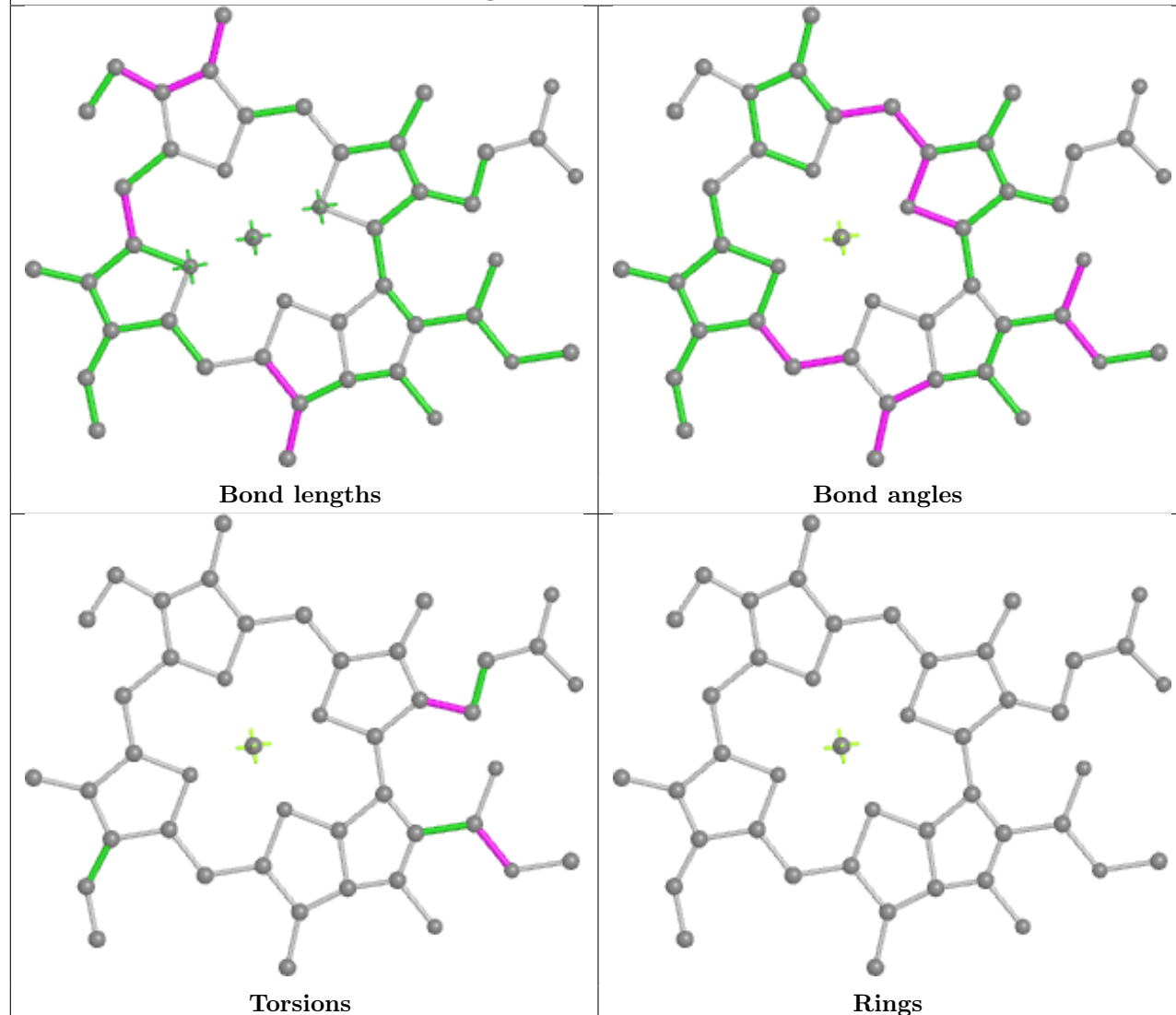
Ligand CLA B2 825



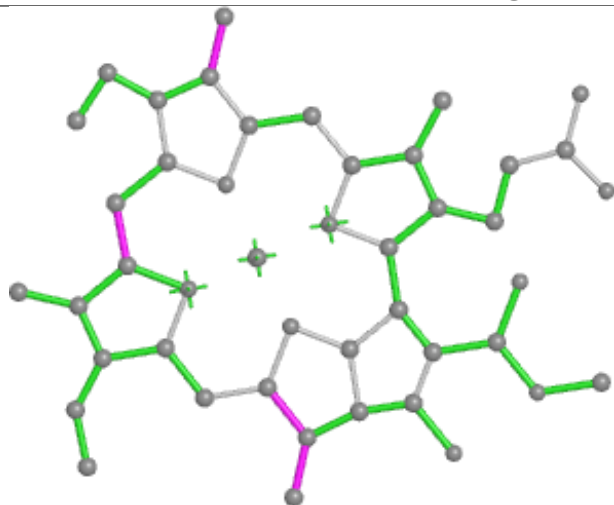
Ligand CLA B2 826



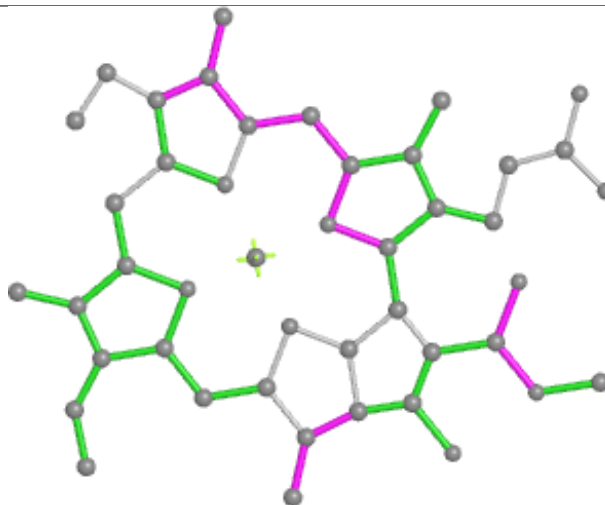
Ligand CLA B2 827



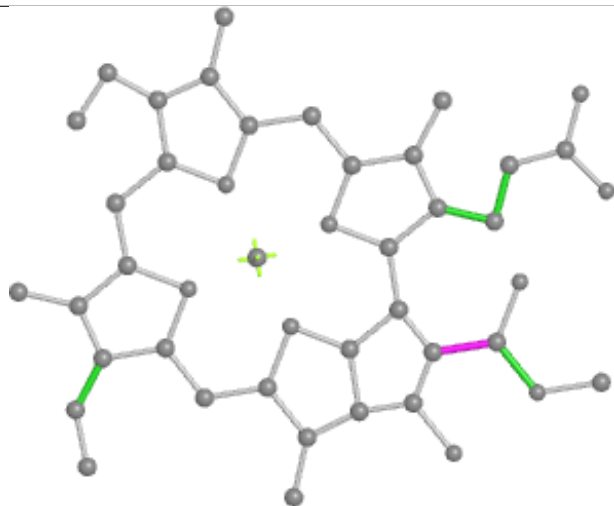
Ligand CLA B2 828



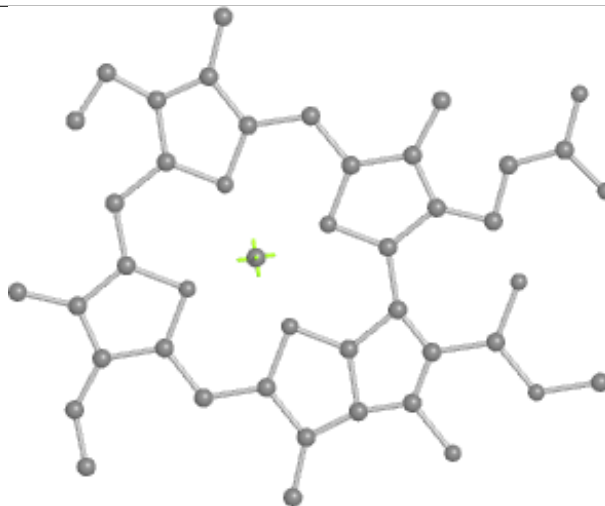
Bond lengths



Bond angles

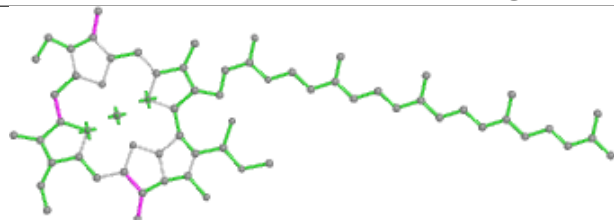


Torsions

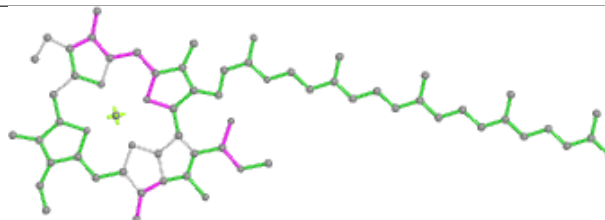


Rings

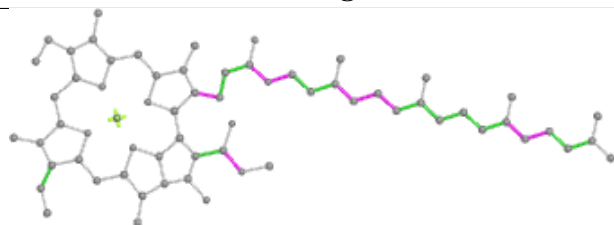
Ligand CLA B2 829



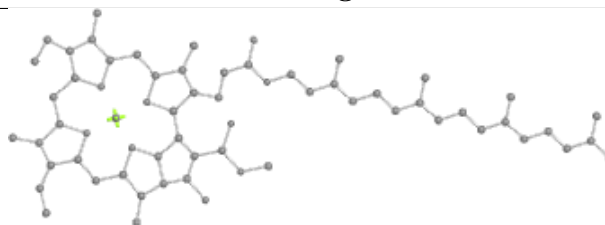
Bond lengths



Bond angles

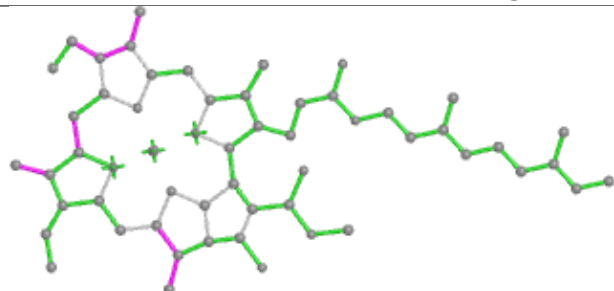


Torsions

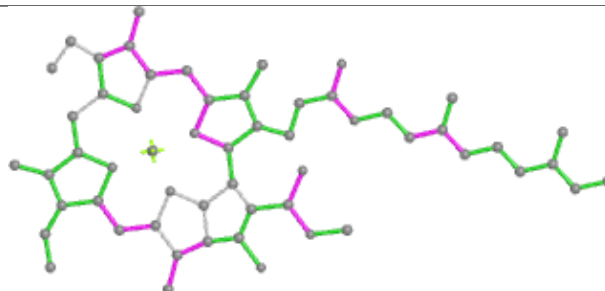


Rings

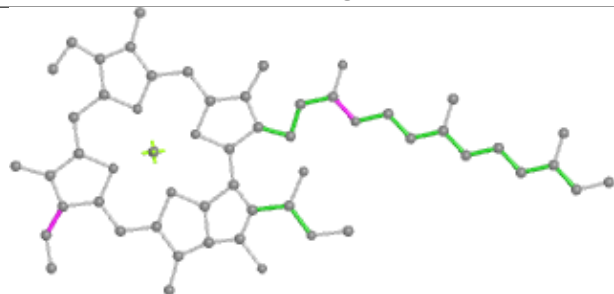
Ligand CLA B2 830



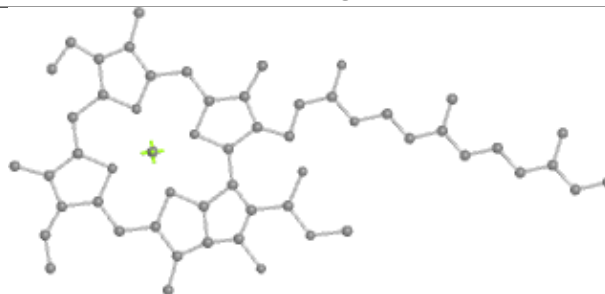
Bond lengths



Bond angles

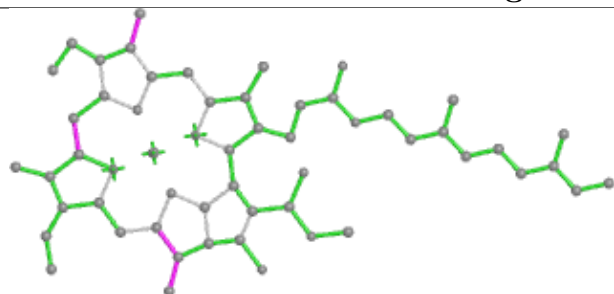


Torsions

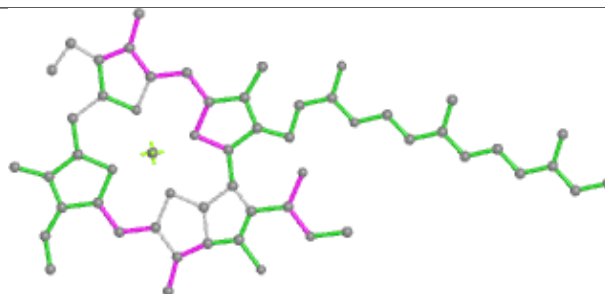


Rings

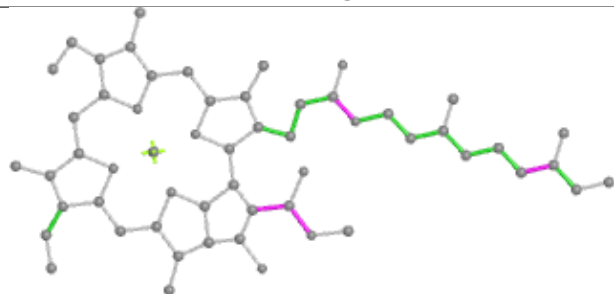
Ligand CLA B2 831



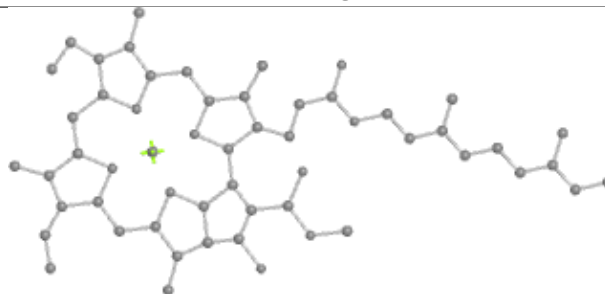
Bond lengths



Bond angles

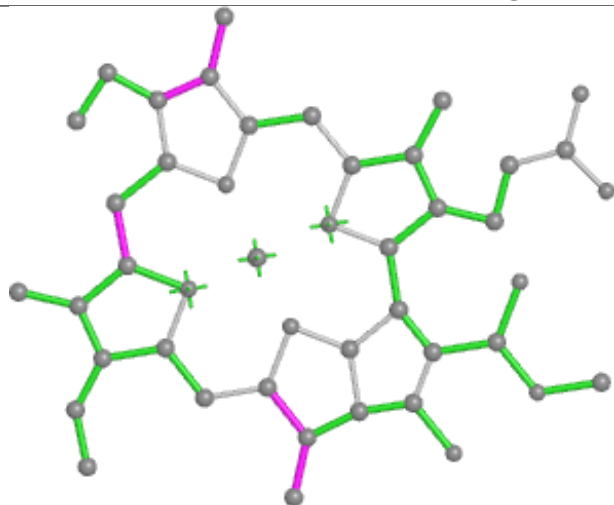


Torsions

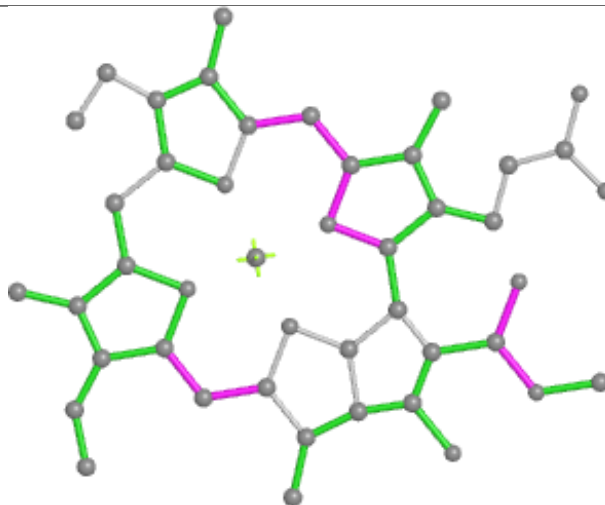


Rings

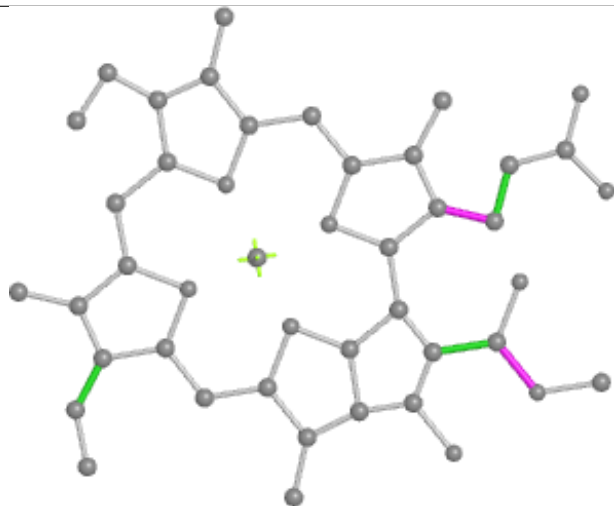
Ligand CLA B2 832



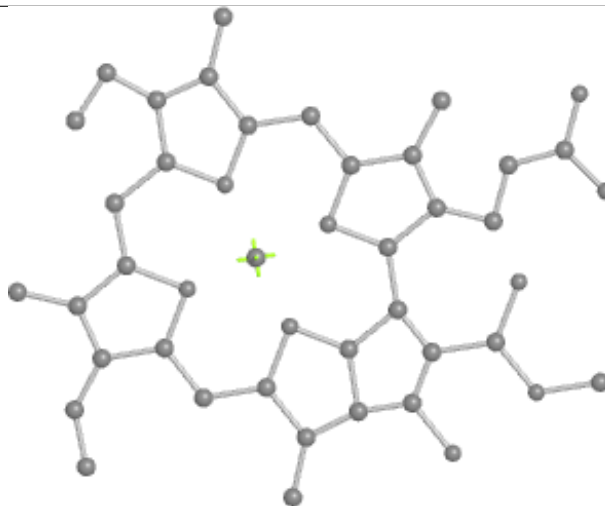
Bond lengths



Bond angles

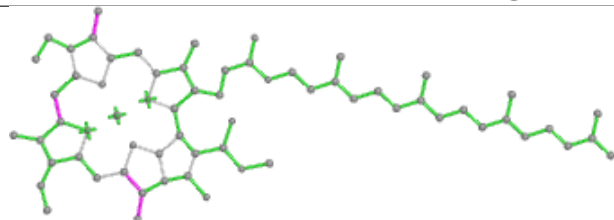


Torsions

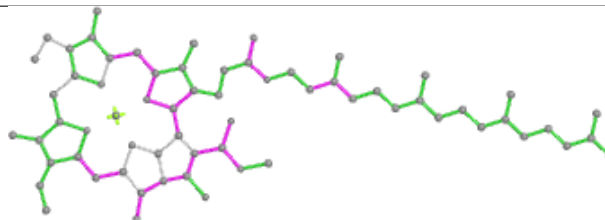


Rings

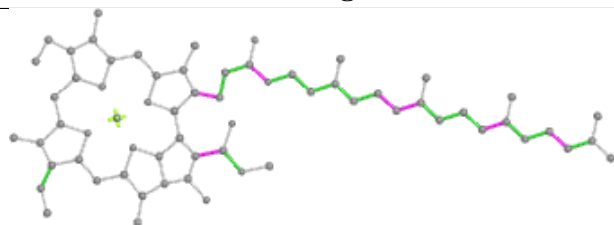
Ligand CLA B2 833



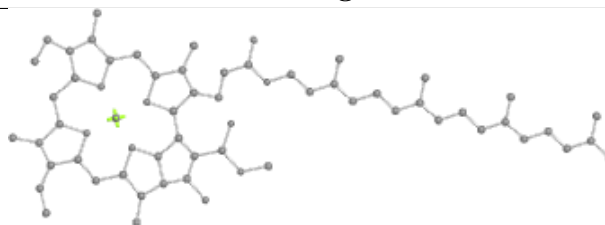
Bond lengths



Bond angles

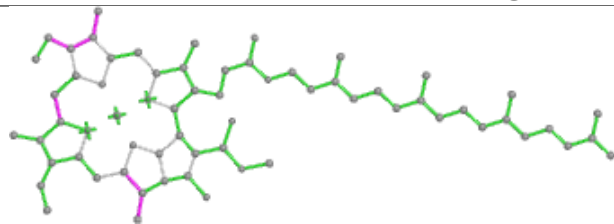


Torsions

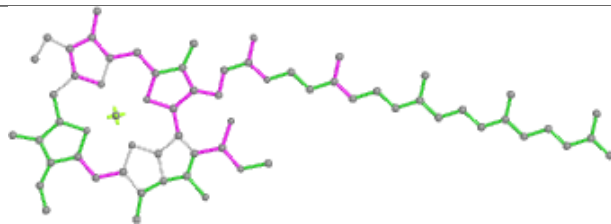


Rings

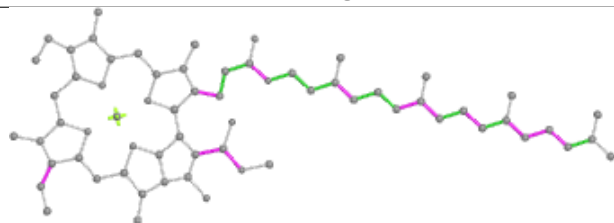
Ligand CLA B2 834



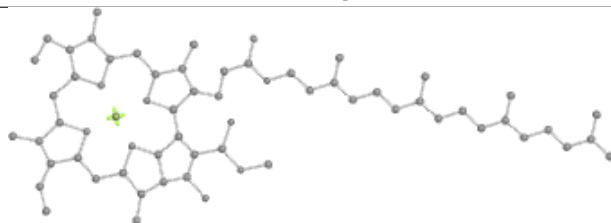
Bond lengths



Bond angles

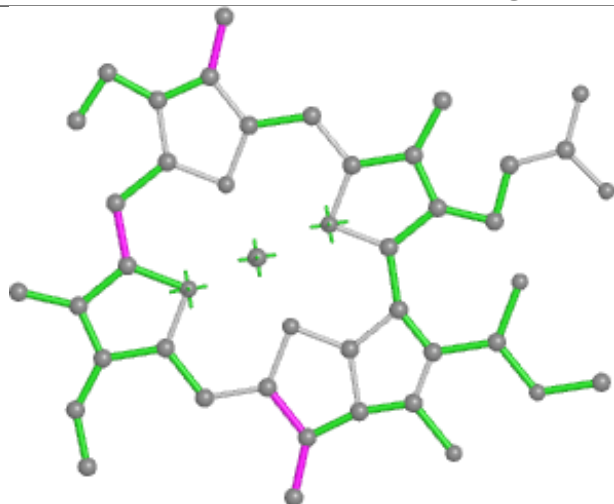


Torsions

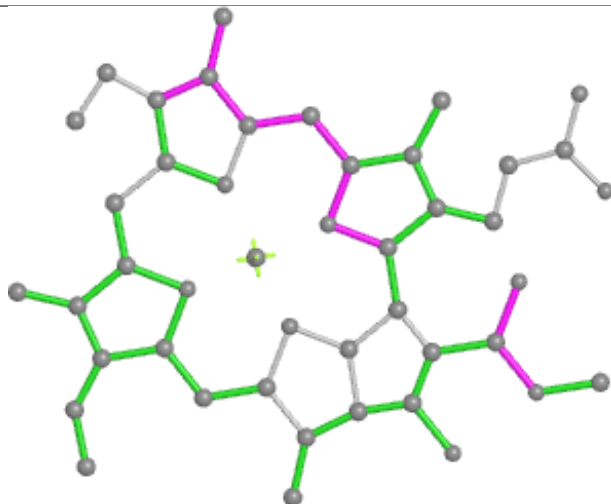


Rings

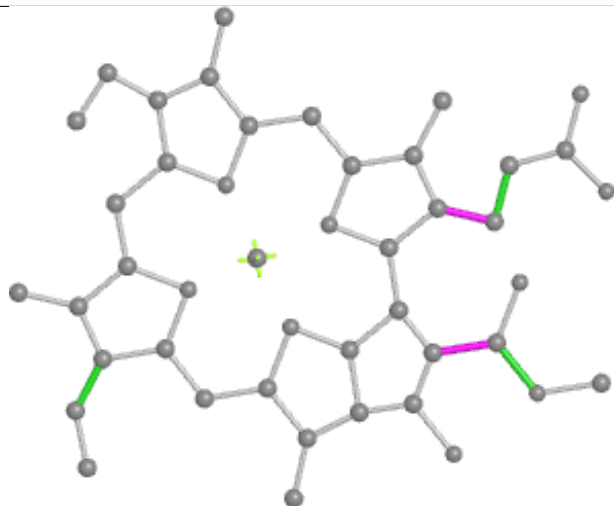
Ligand CLA B2 835



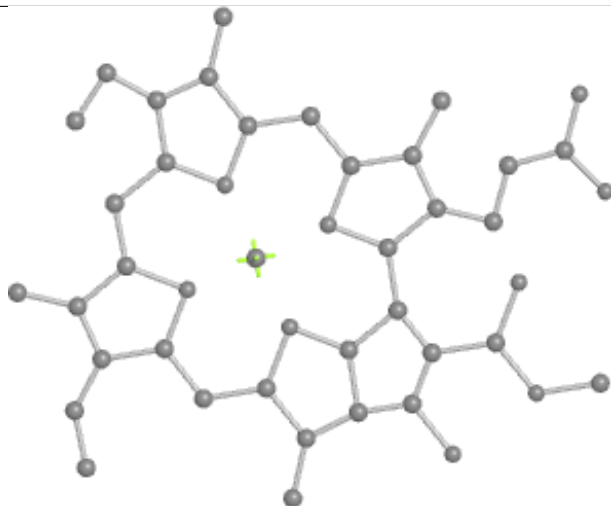
Bond lengths



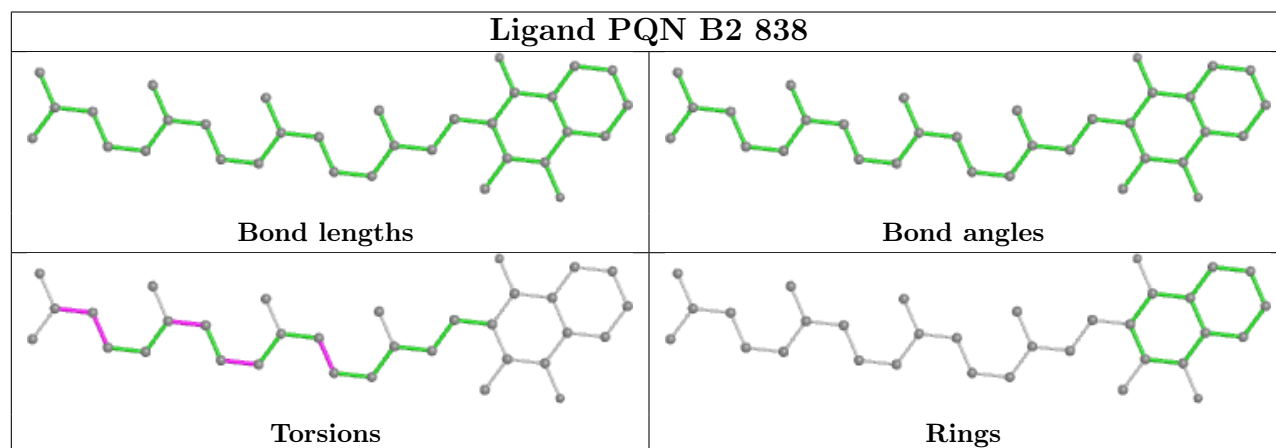
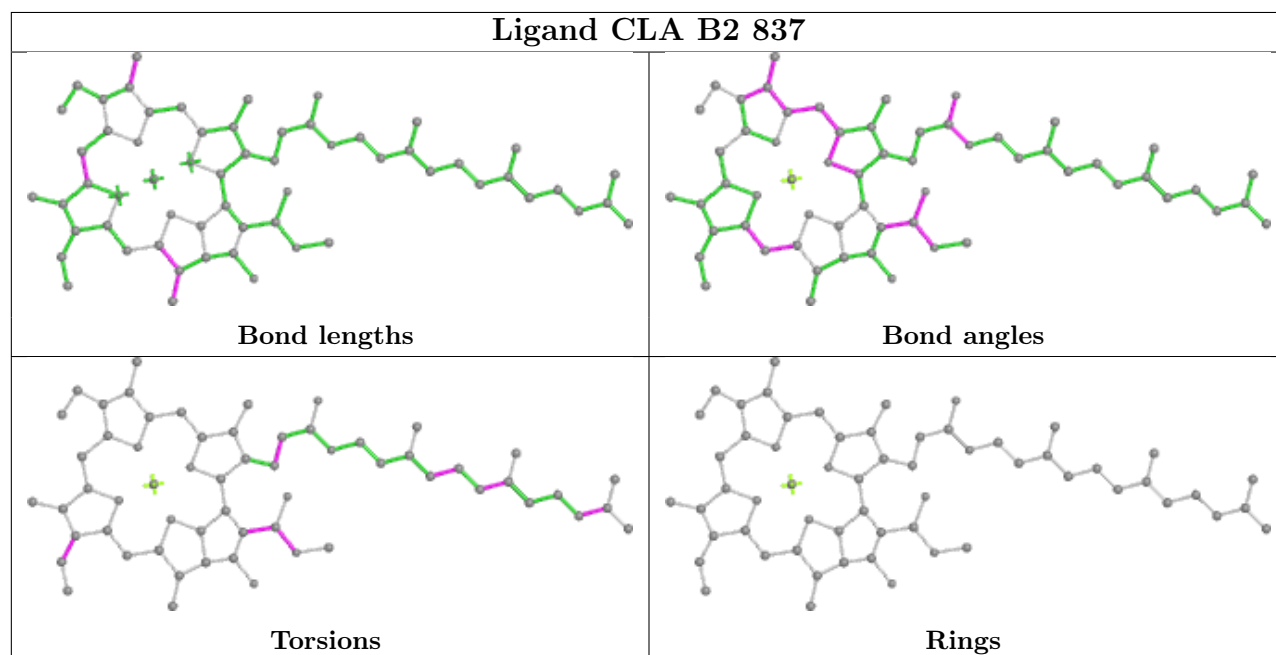
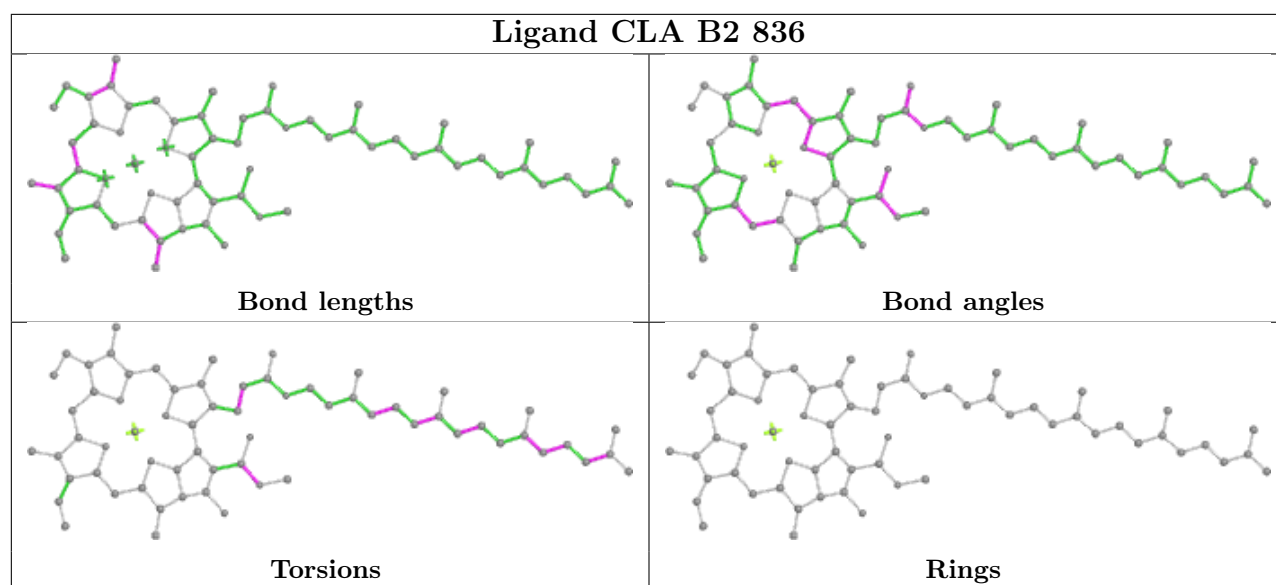
Bond angles

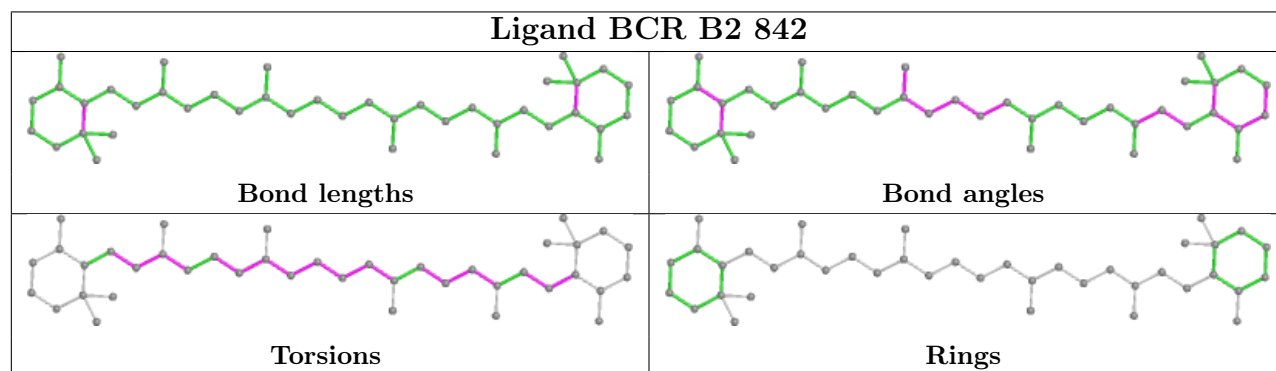
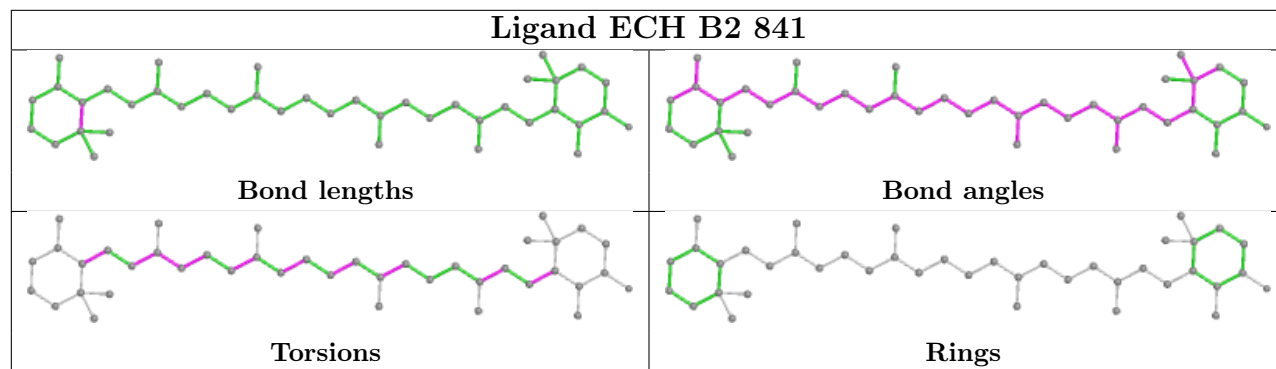
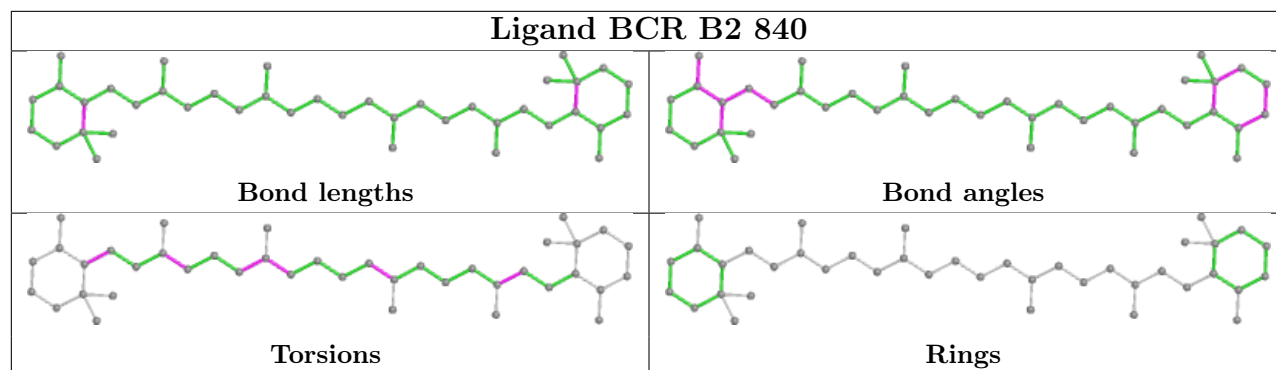
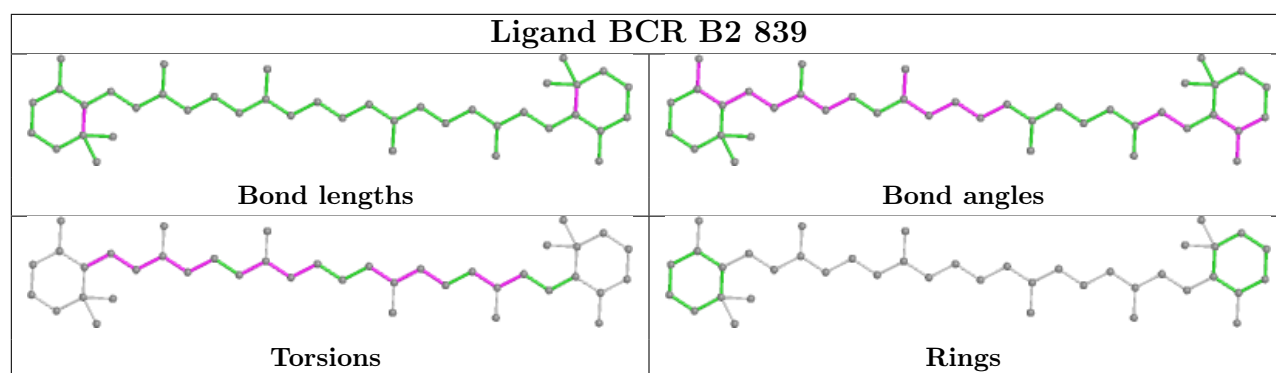


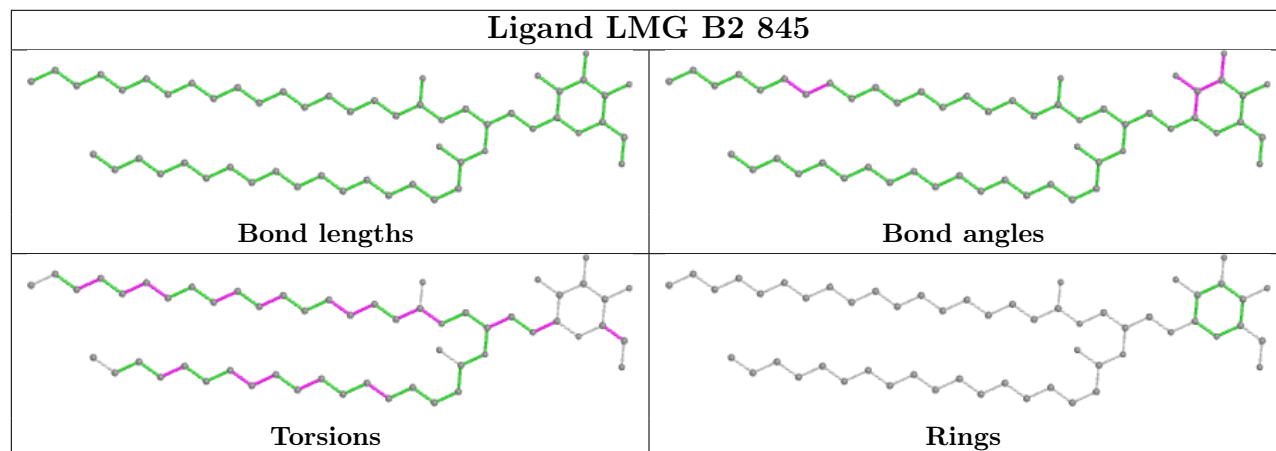
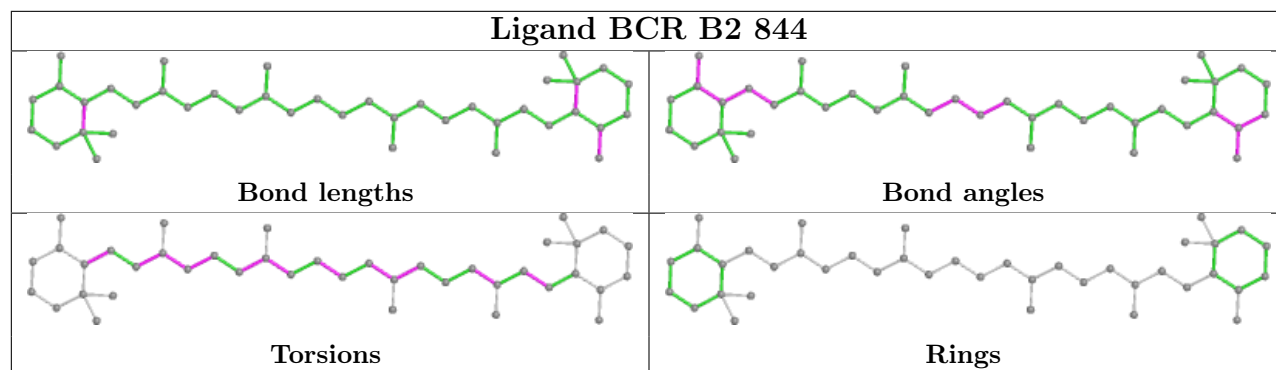
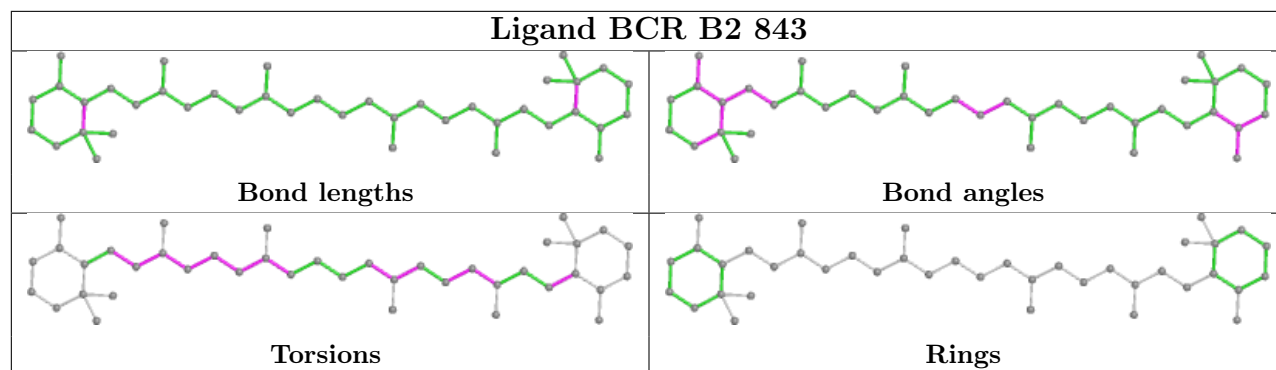
Torsions



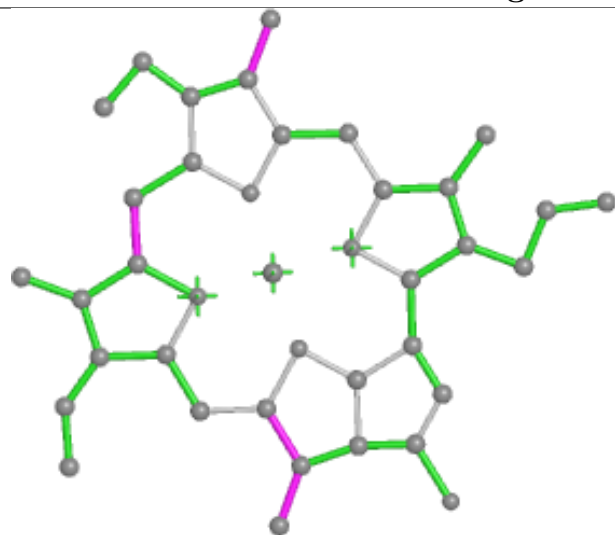
Rings



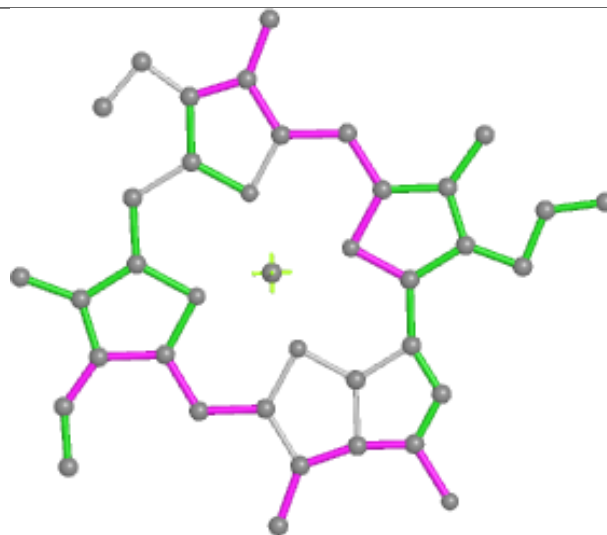




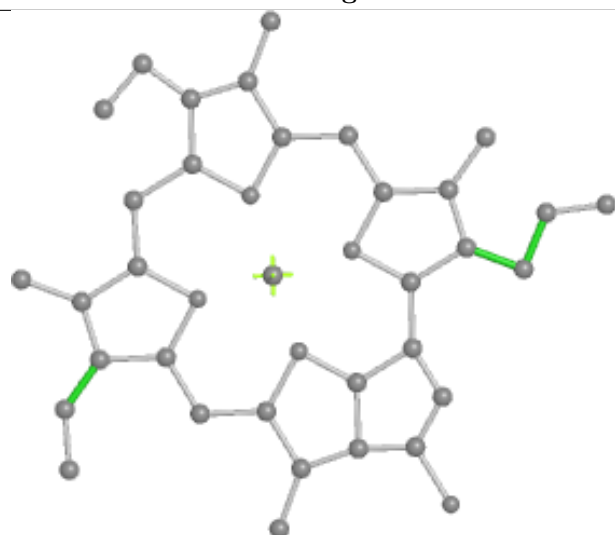
Ligand CLA B2 846



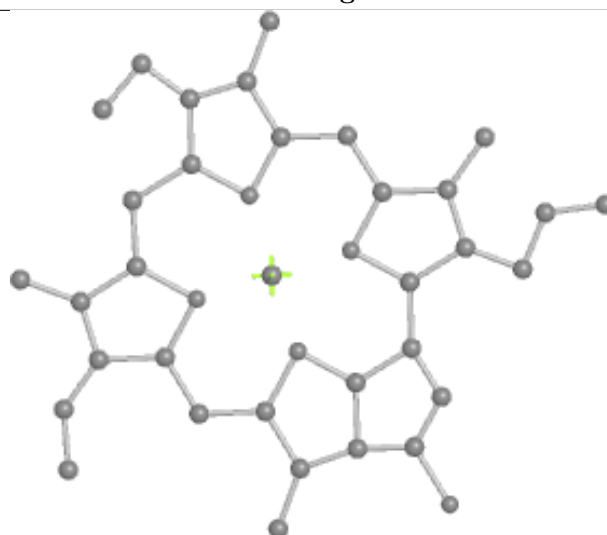
Bond lengths



Bond angles

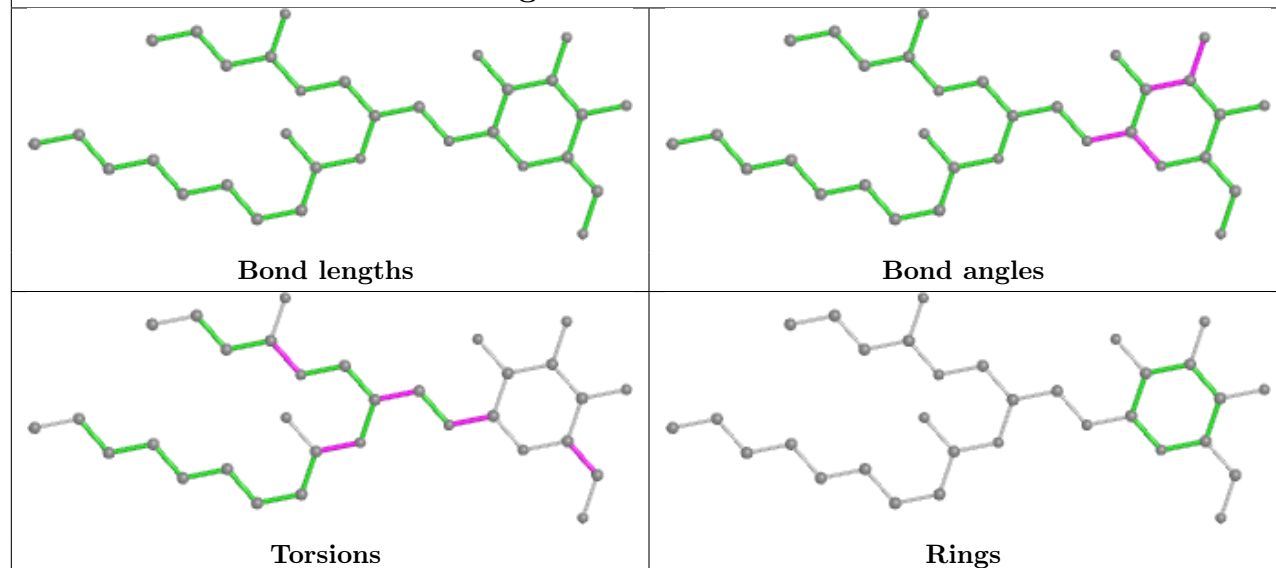


Torsions

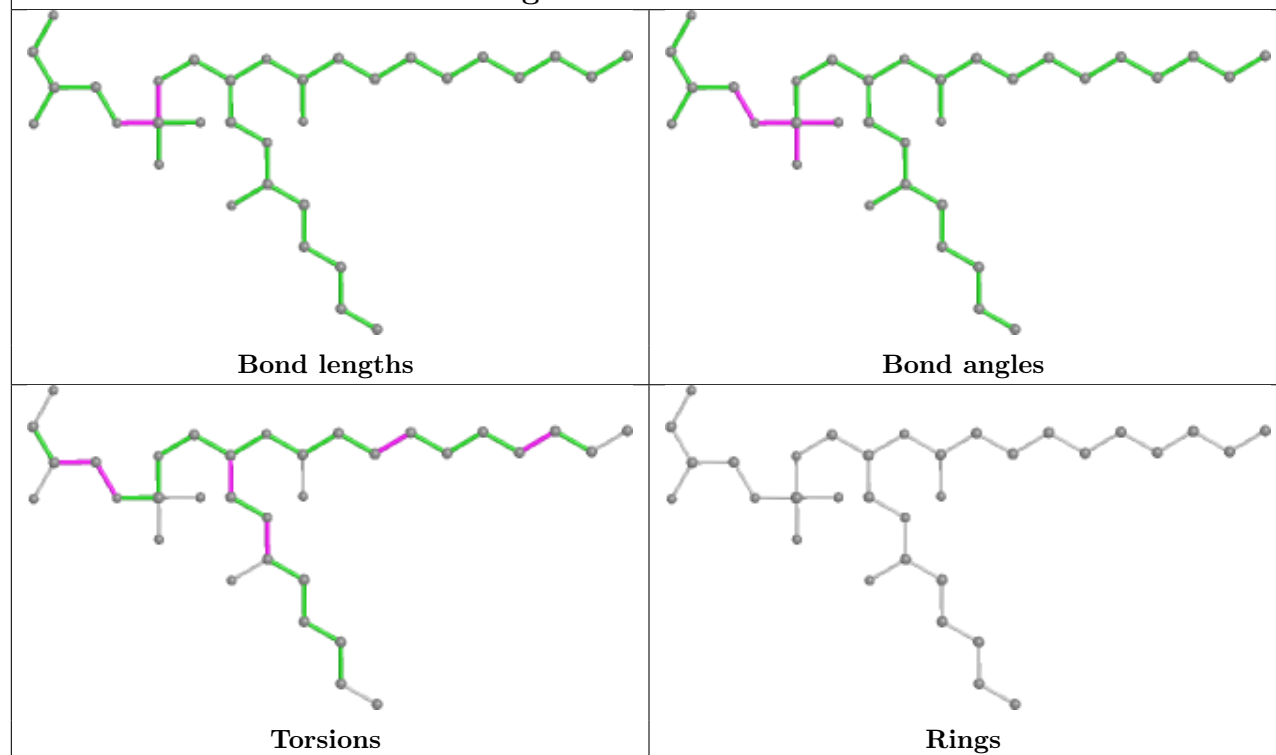


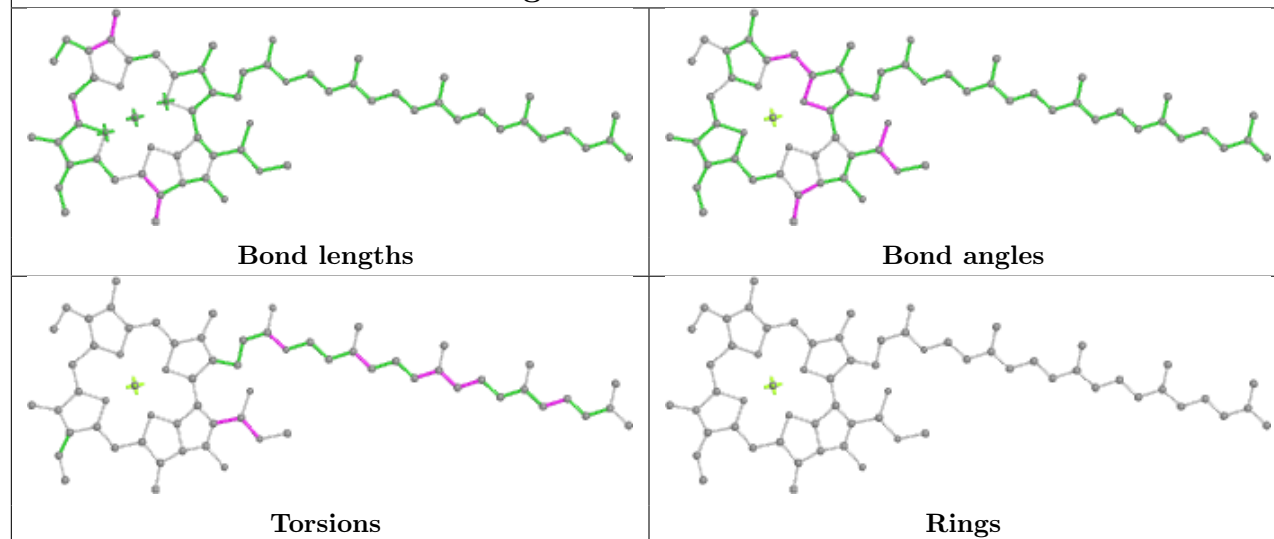
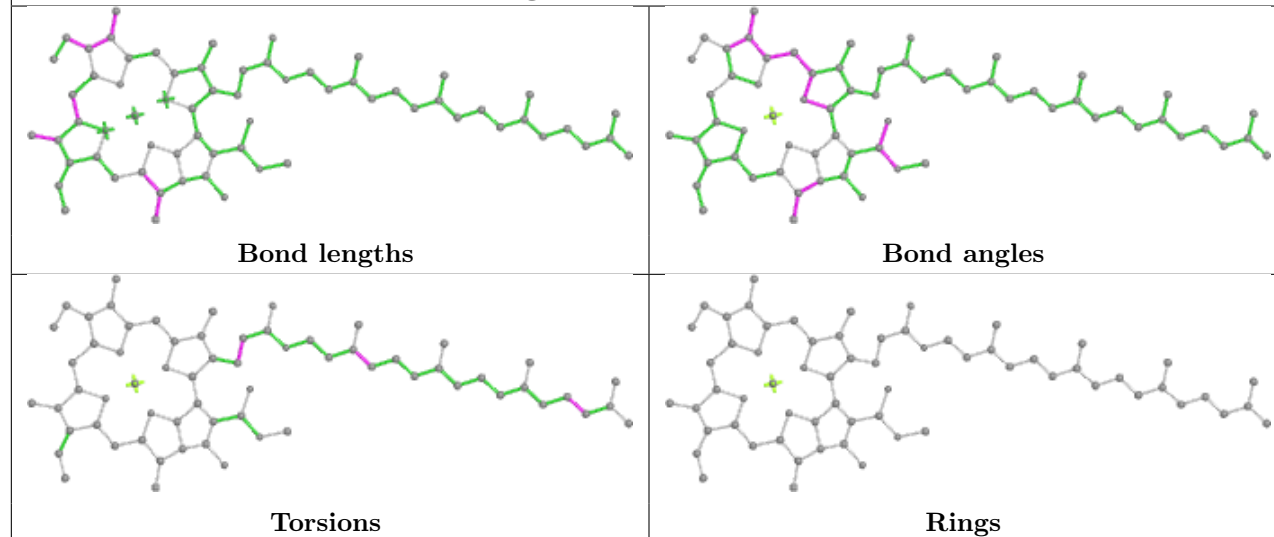
Rings

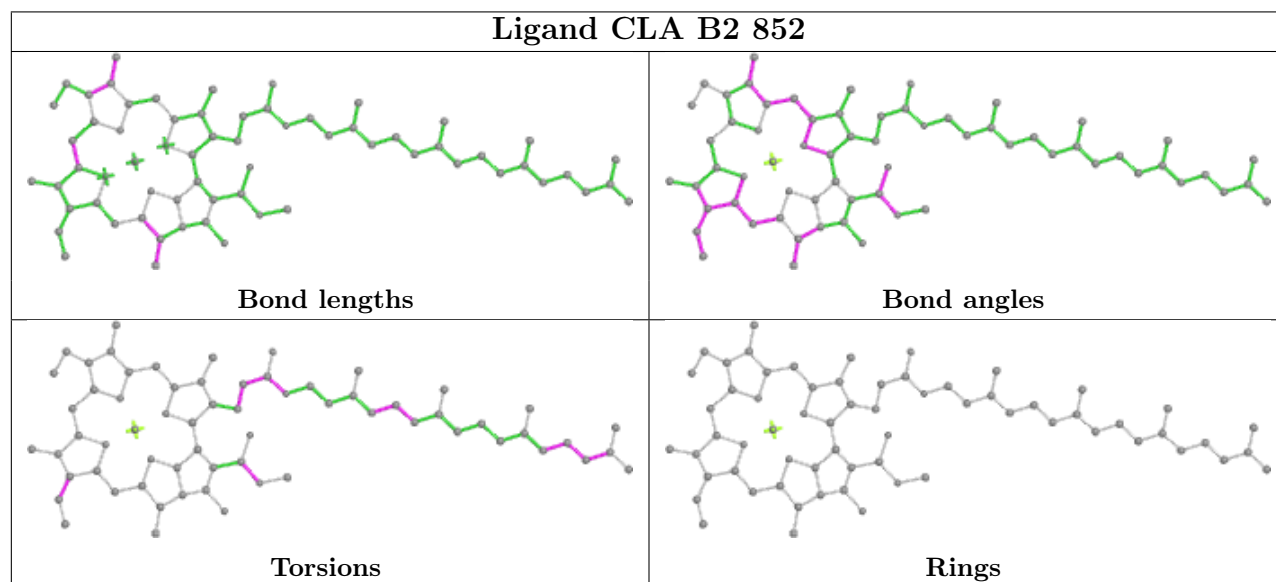
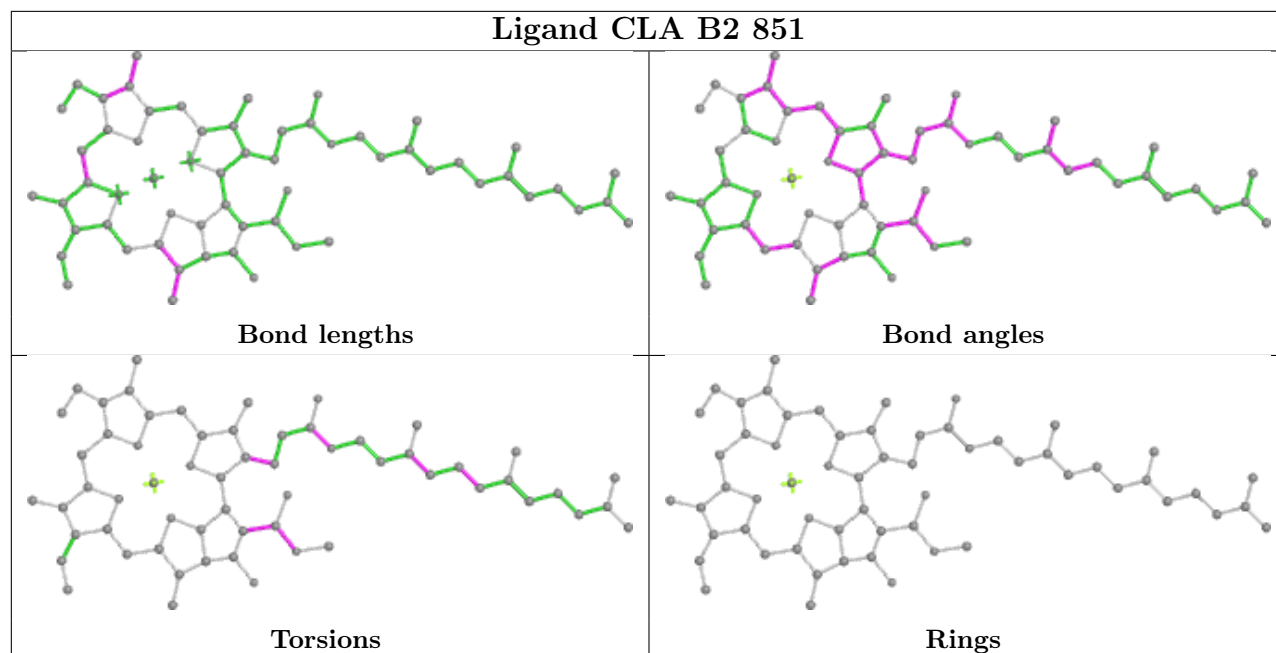
Ligand LMG B2 847



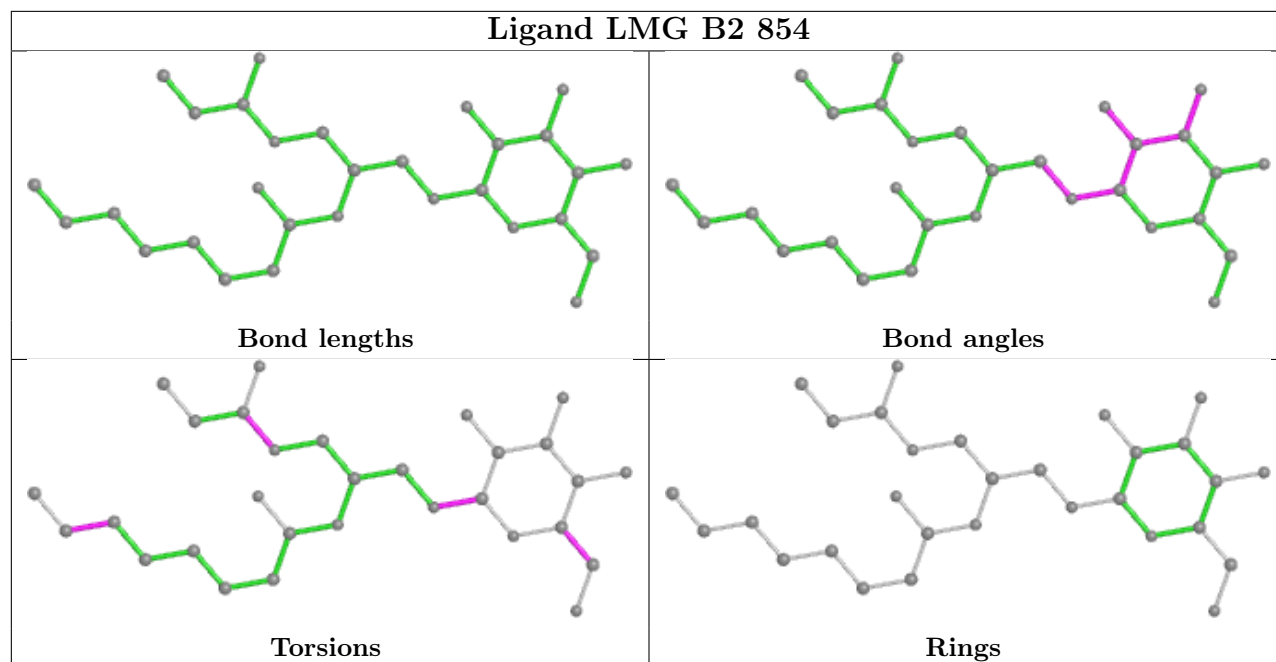
Ligand LHG B2 848



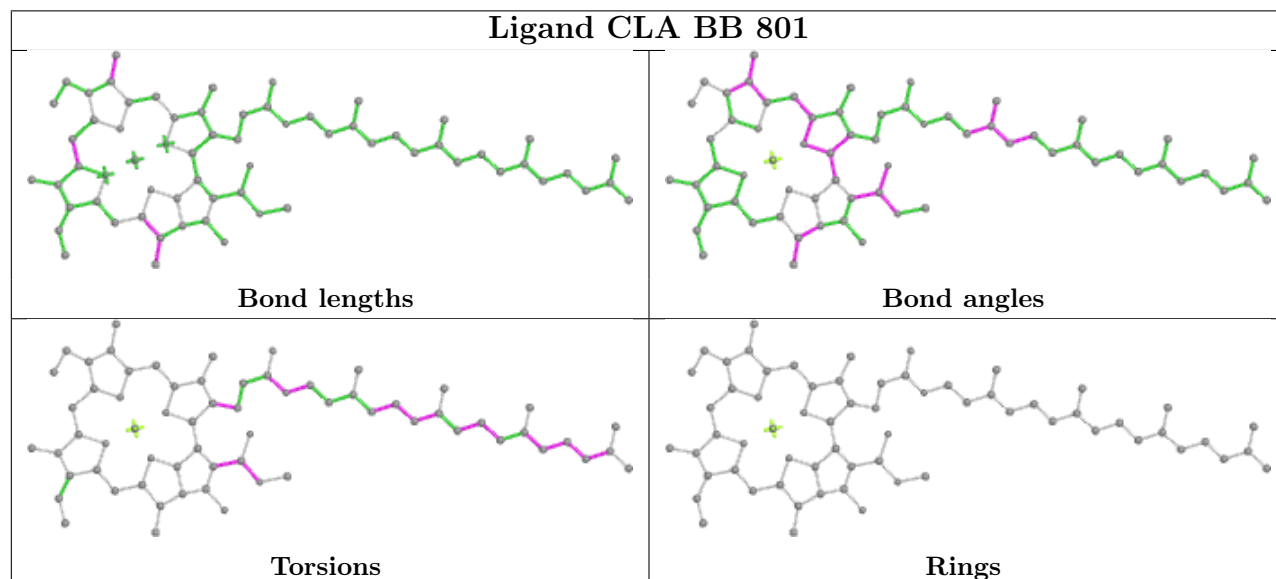
Ligand CLA B2 849**Ligand CLA B2 850**



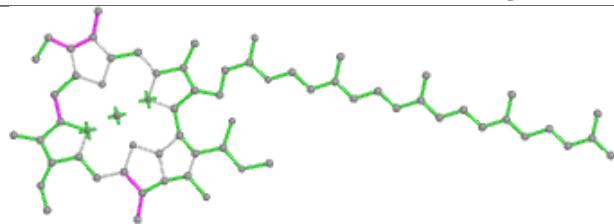
Ligand LMG B2 854



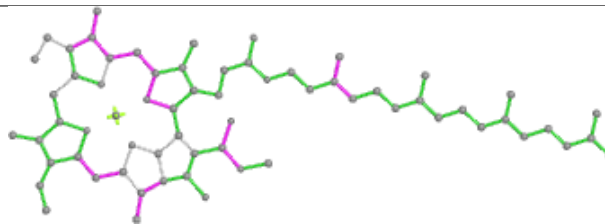
Ligand CLA BB 801



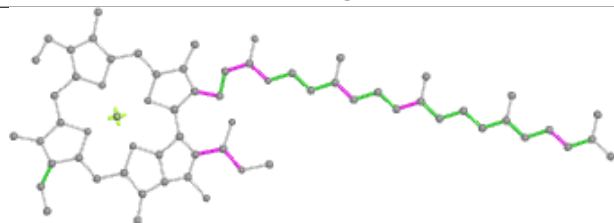
Ligand CLA BB 802



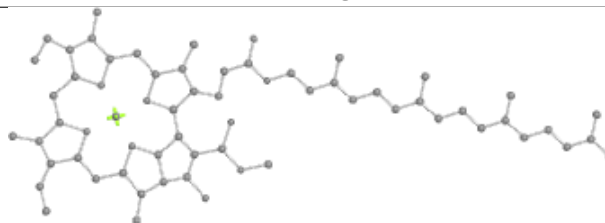
Bond lengths



Bond angles

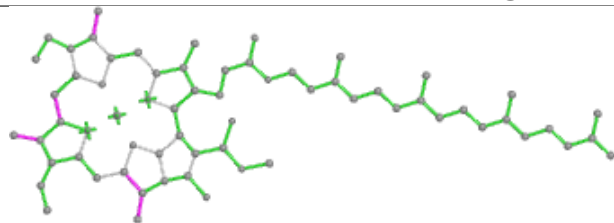


Torsions

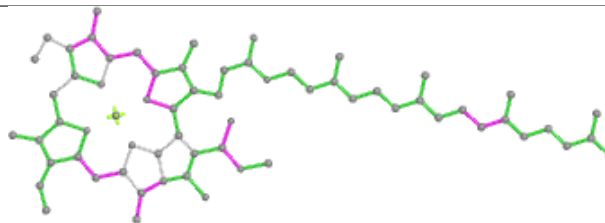


Rings

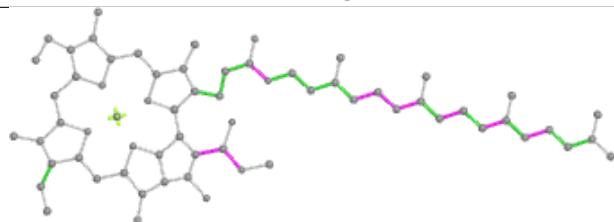
Ligand CLA BB 803



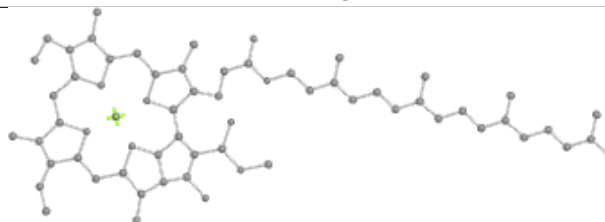
Bond lengths



Bond angles

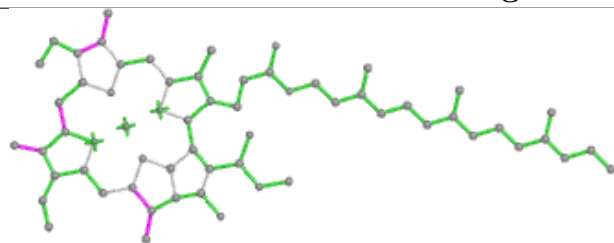


Torsions

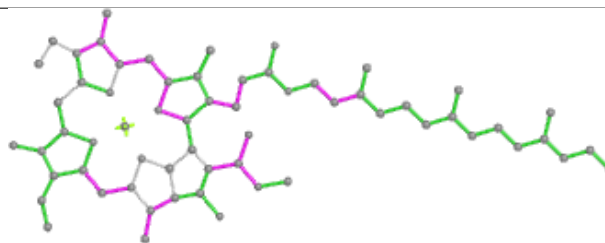


Rings

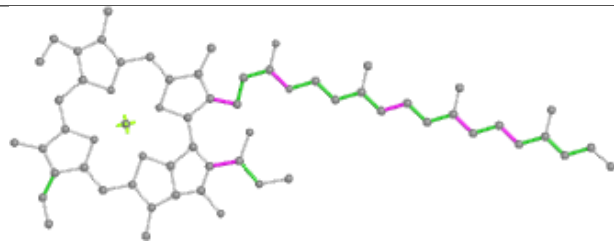
Ligand CLA BB 804



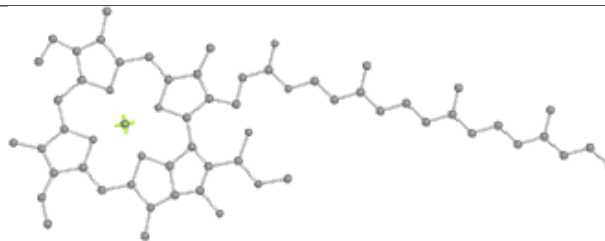
Bond lengths



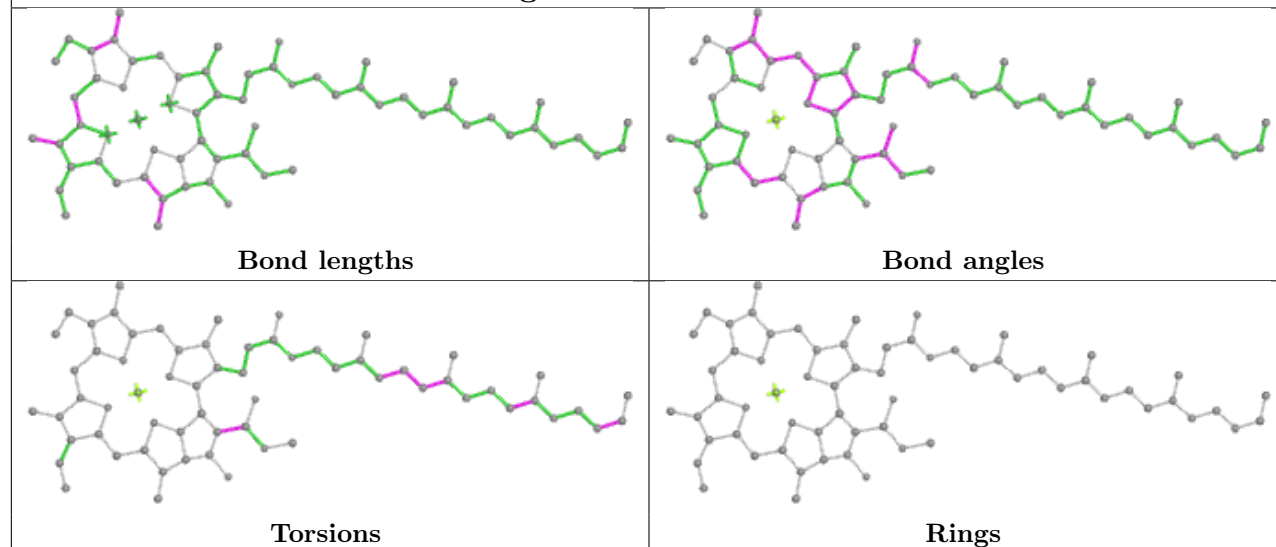
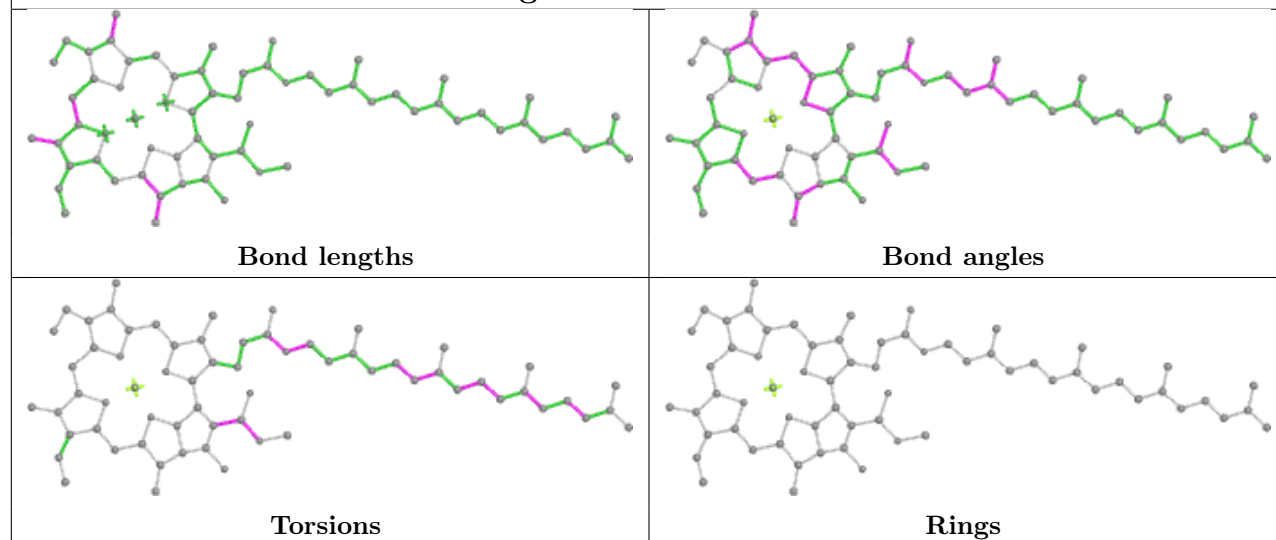
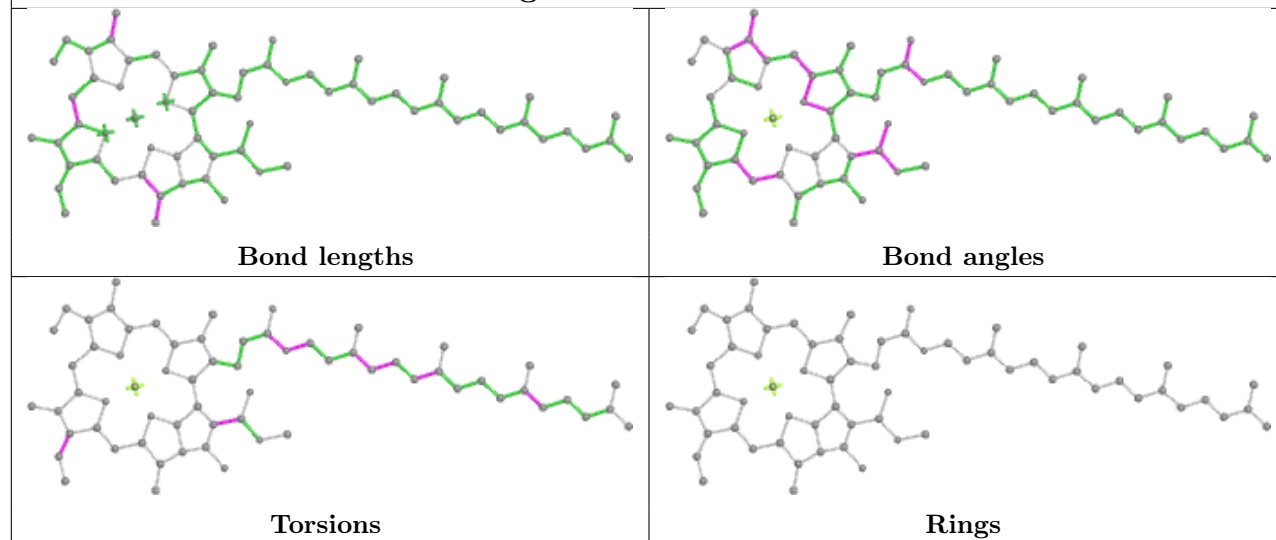
Bond angles



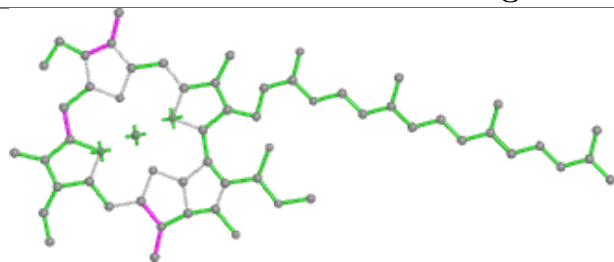
Torsions



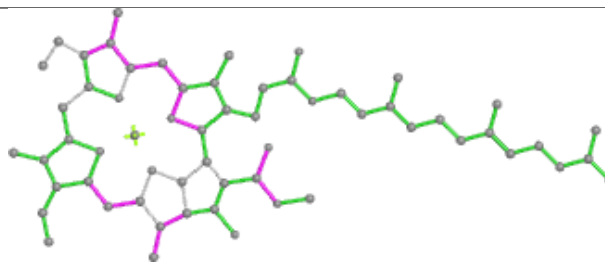
Rings

Ligand CLA BB 805**Ligand CLA BB 806****Ligand CLA BB 807**

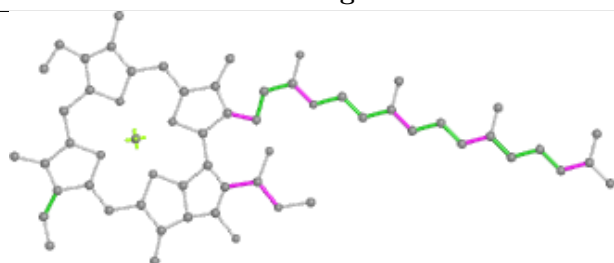
Ligand CLA BB 808



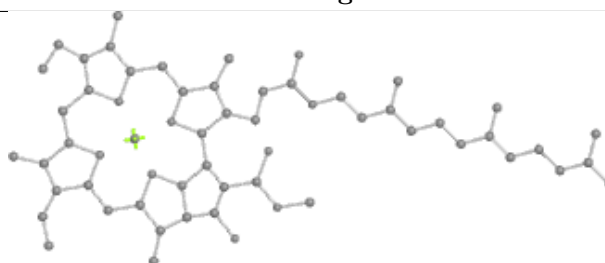
Bond lengths



Bond angles

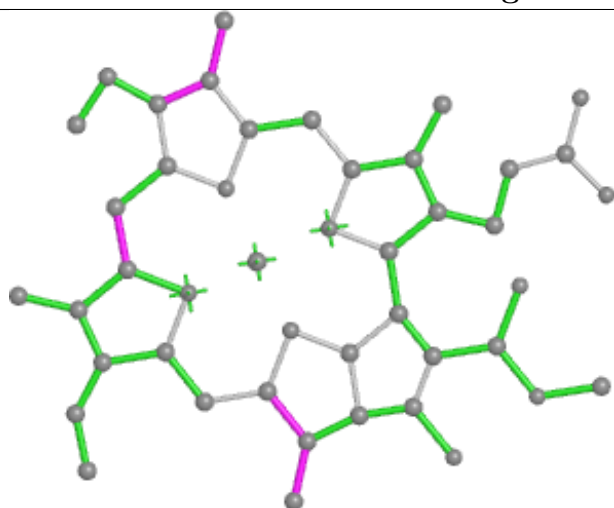


Torsions

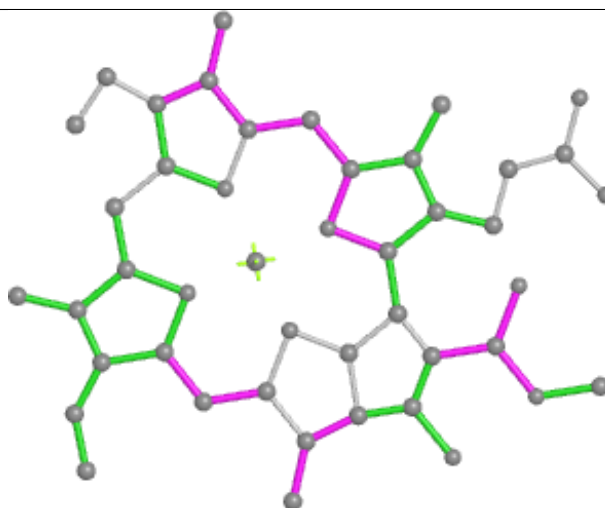


Rings

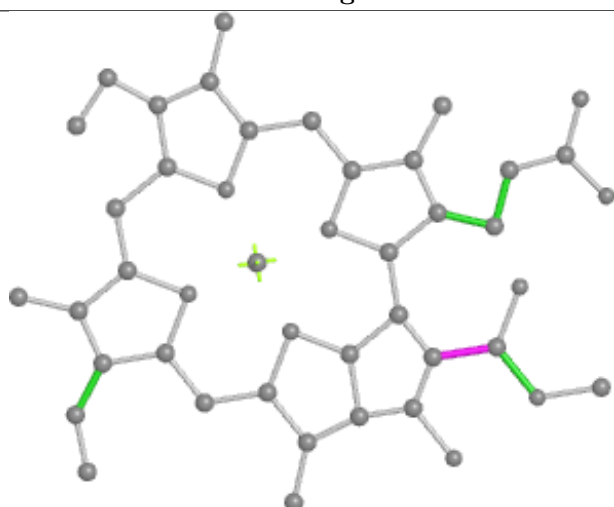
Ligand CLA BB 809



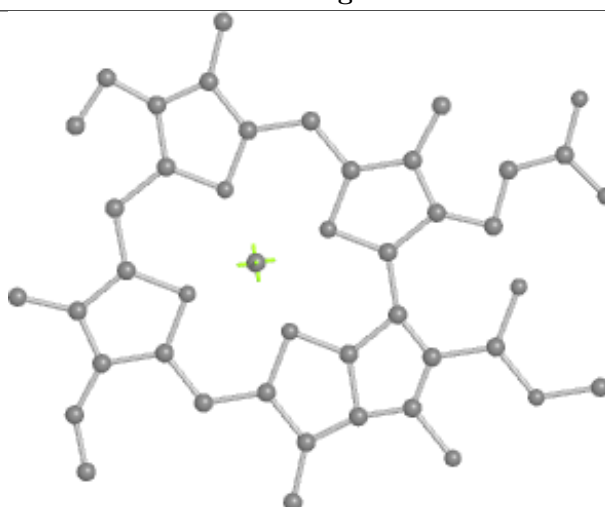
Bond lengths



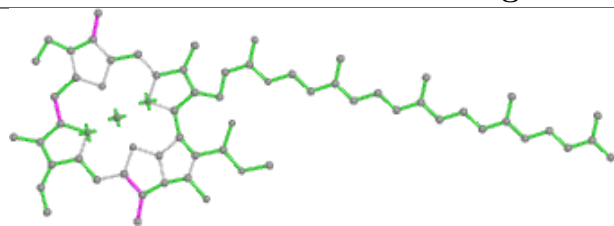
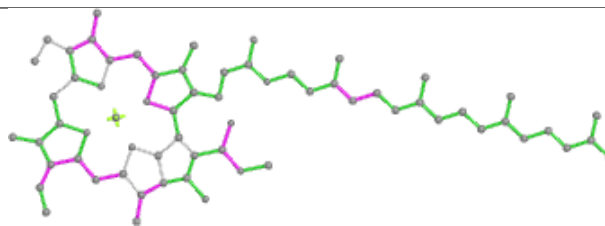
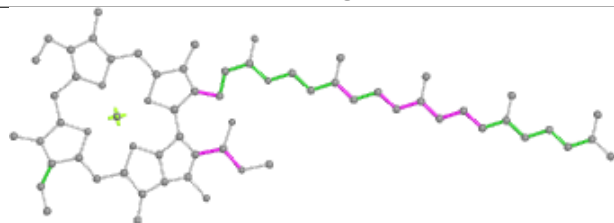
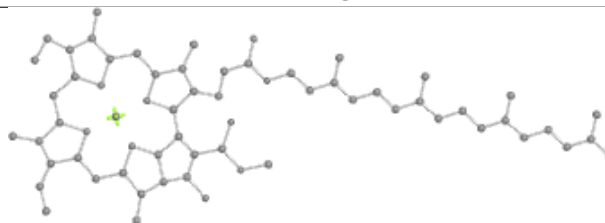
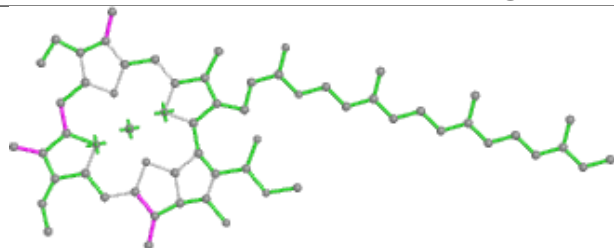
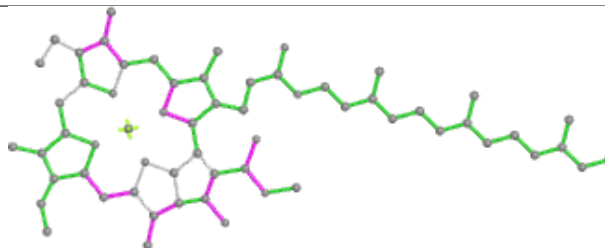
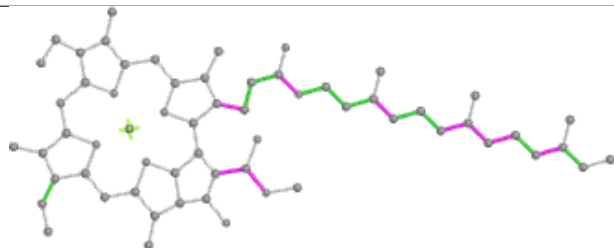
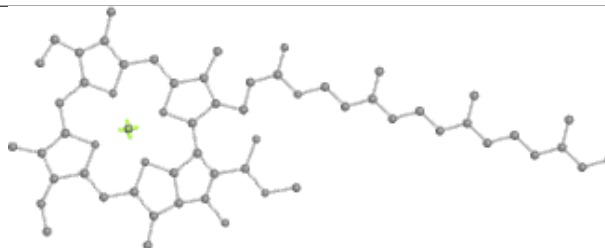
Bond angles



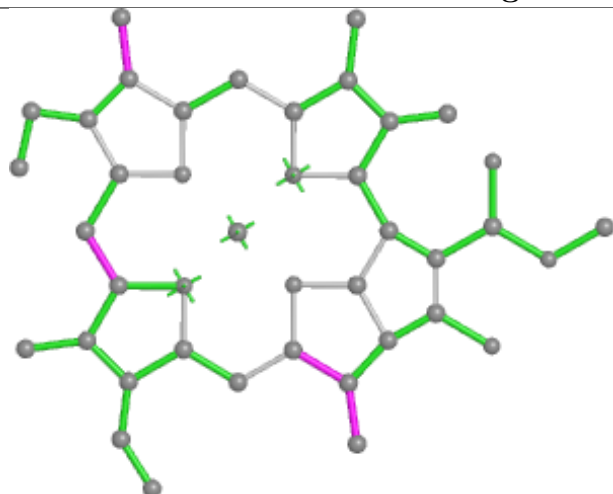
Torsions



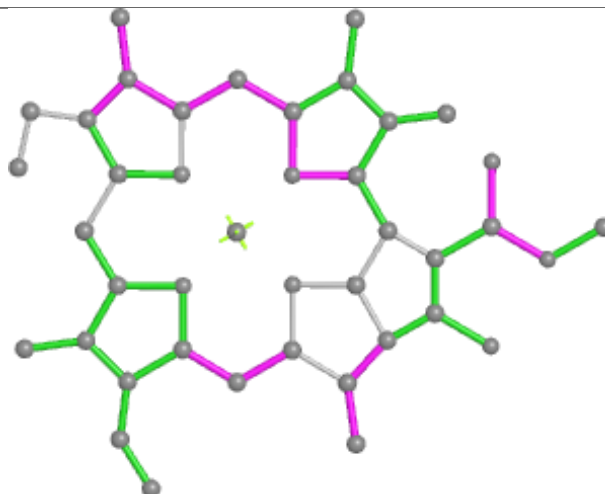
Rings

Ligand CLA BB 810**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA BB 811****Bond lengths****Bond angles****Torsions****Rings**

Ligand CLA BB 812



Bond lengths



Bond angles

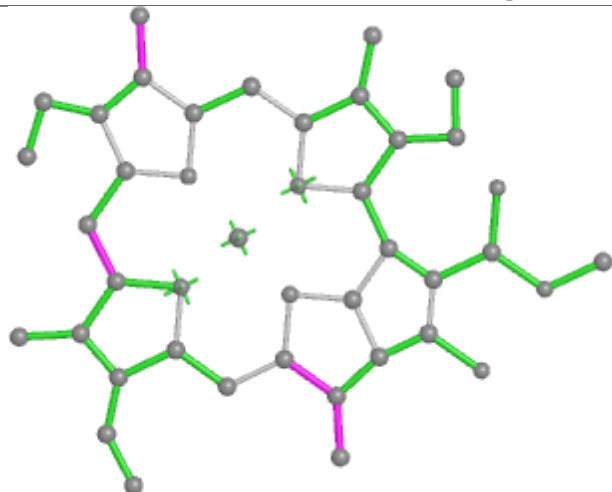


Torsions

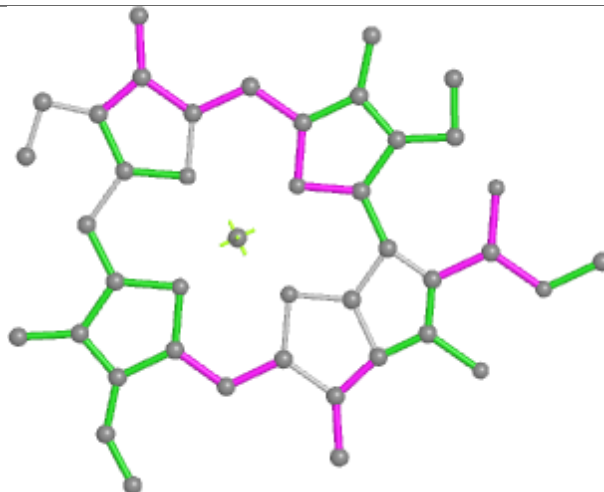


Rings

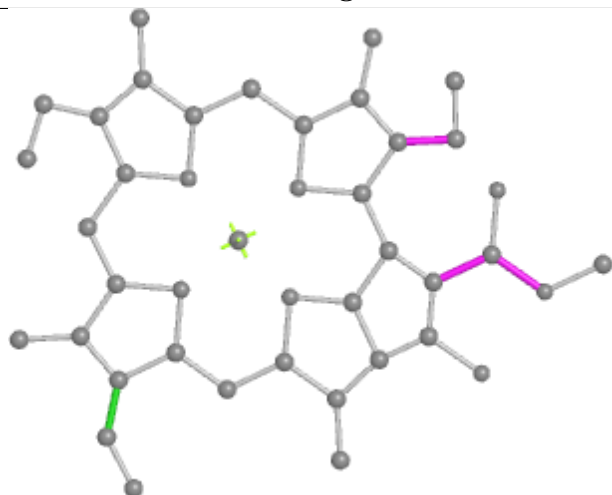
Ligand CLA BB 813



Bond lengths



Bond angles

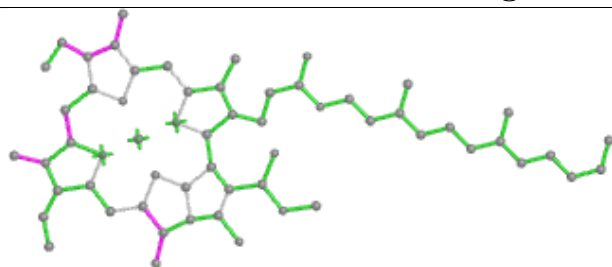


Torsions

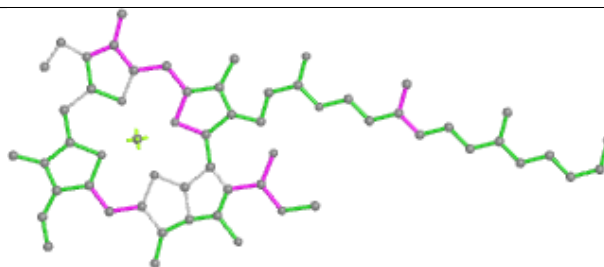


Rings

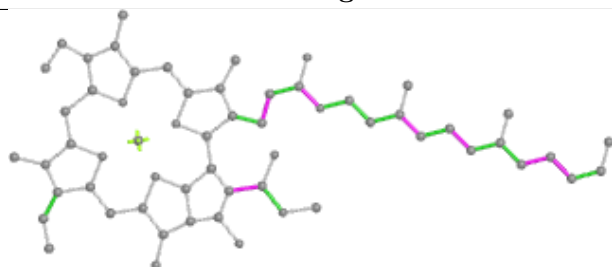
Ligand CLA BB 814



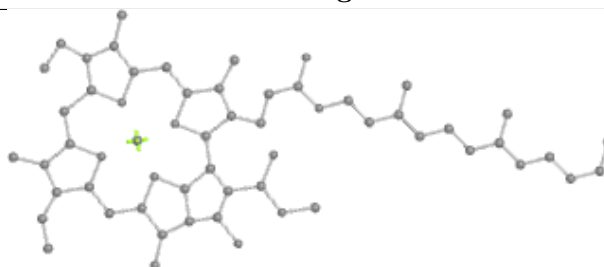
Bond lengths



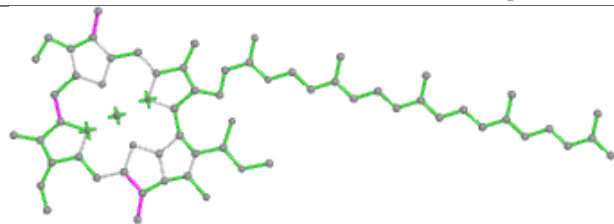
Bond angles



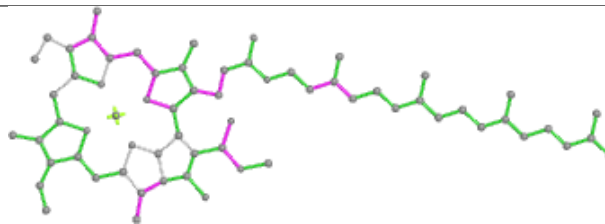
Torsions



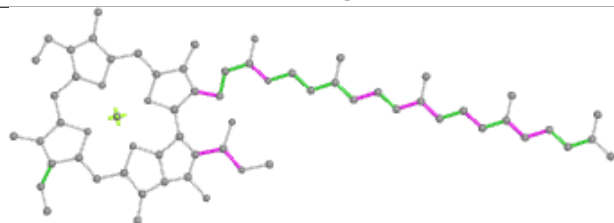
Rings

Ligand CLA BB 815

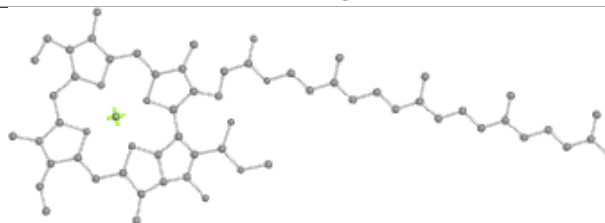
Bond lengths



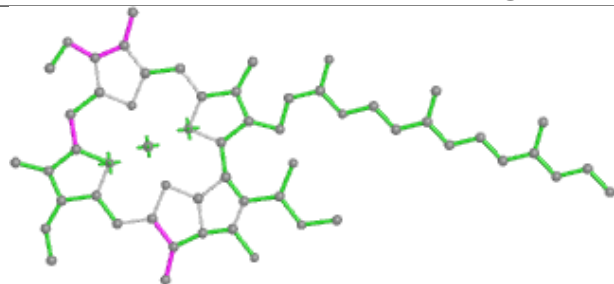
Bond angles



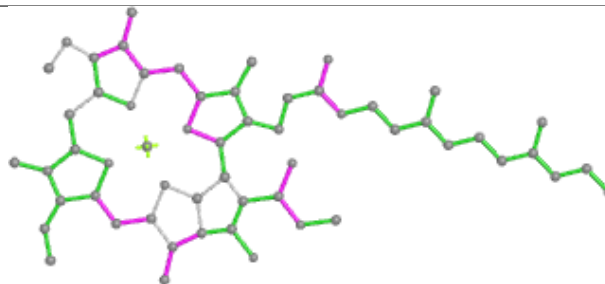
Torsions



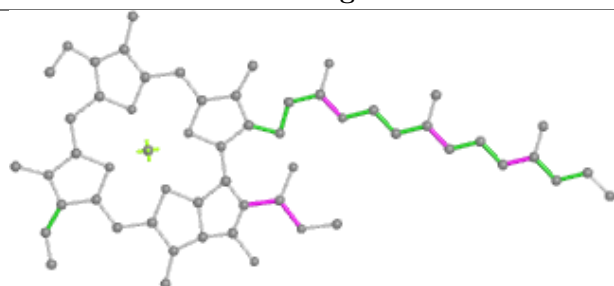
Rings

Ligand CLA BB 816

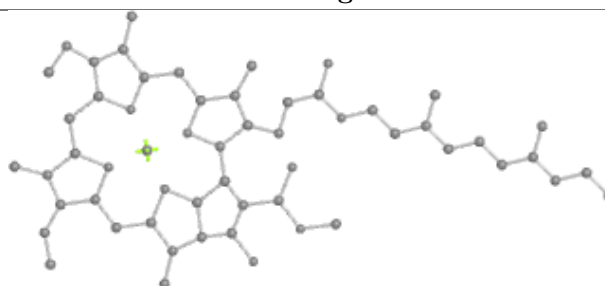
Bond lengths



Bond angles

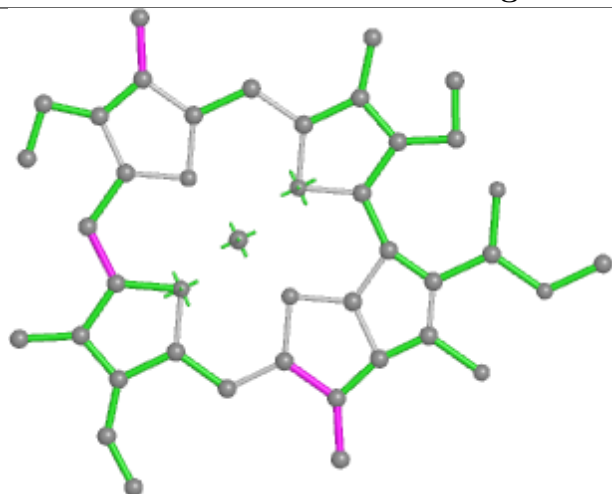


Torsions

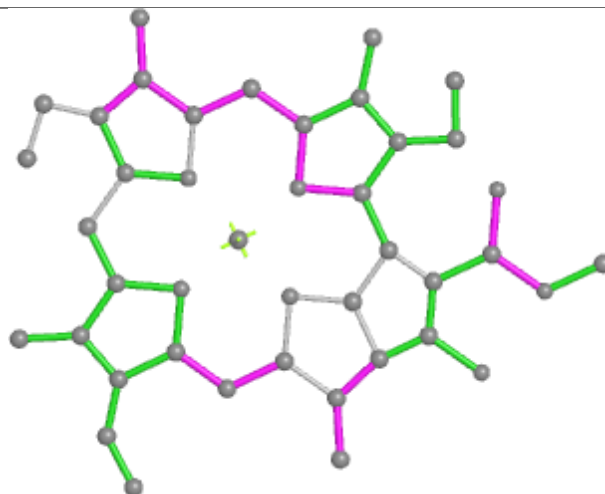


Rings

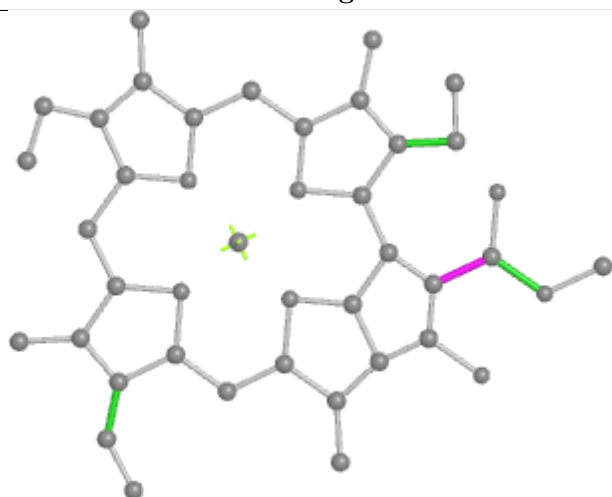
Ligand CLA BB 817



Bond lengths



Bond angles

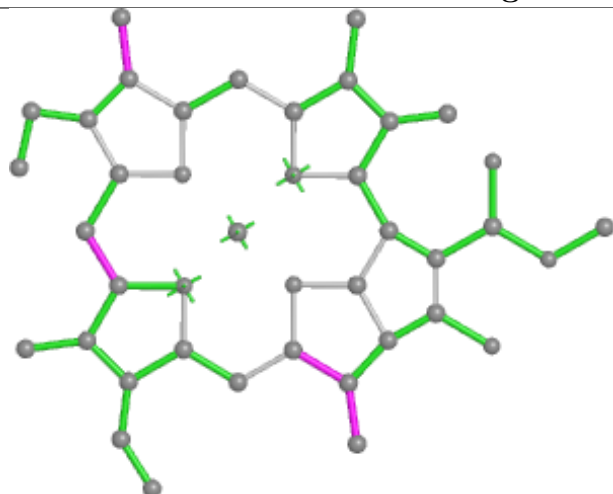


Torsions

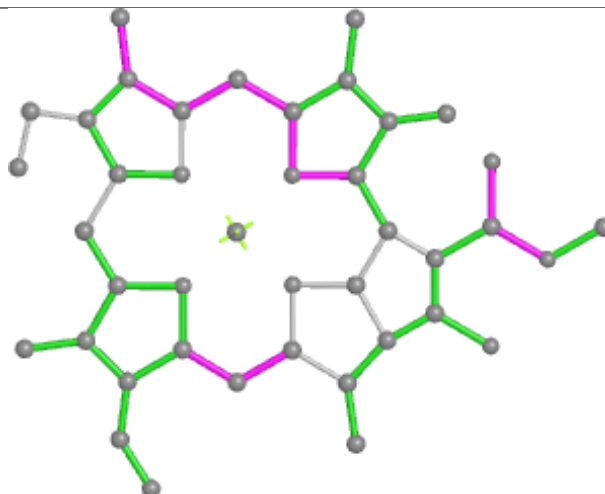


Rings

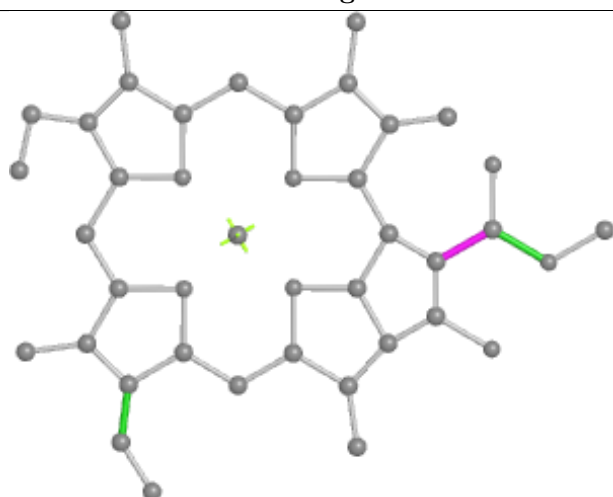
Ligand CLA BB 818



Bond lengths



Bond angles

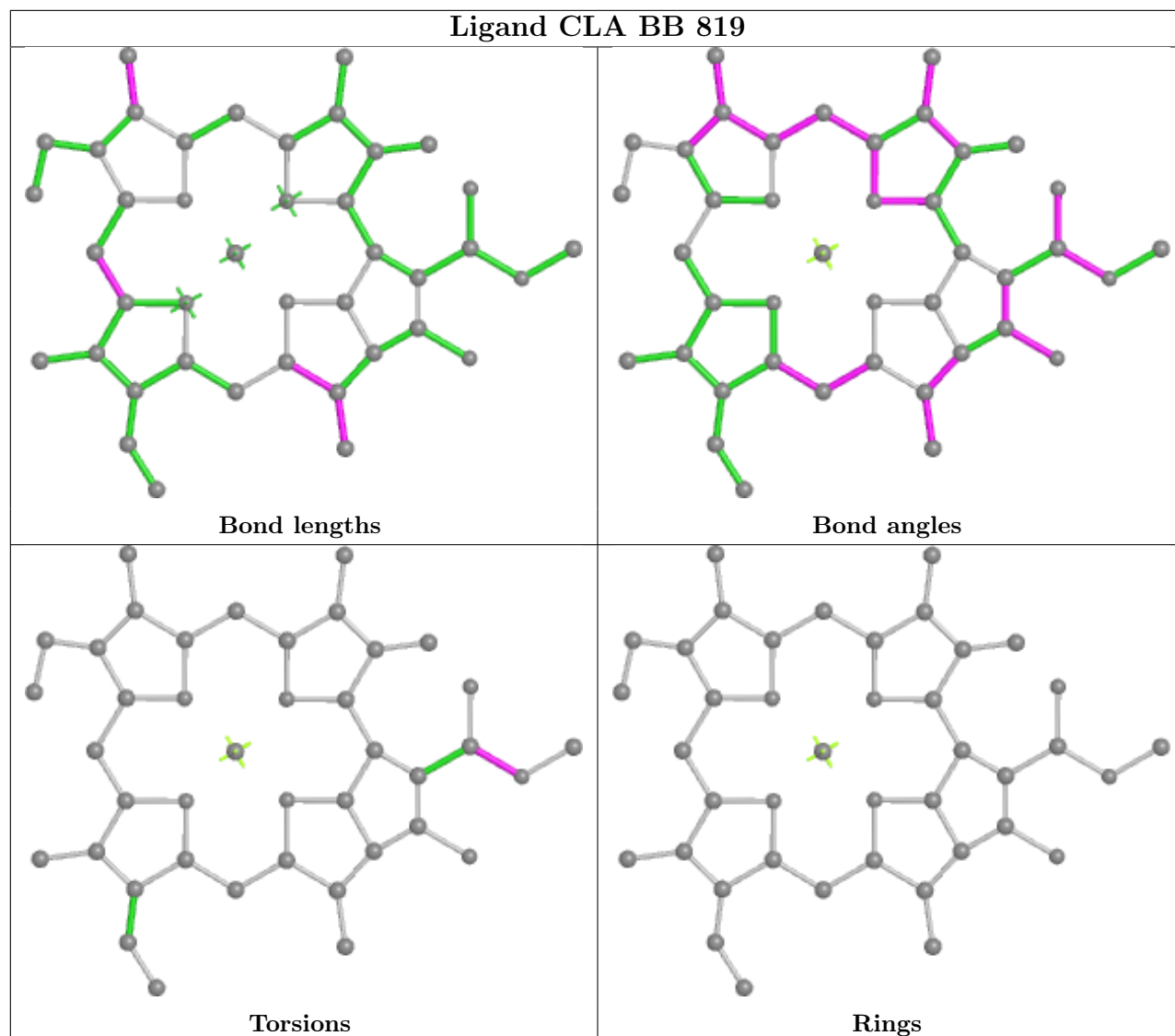


Torsions

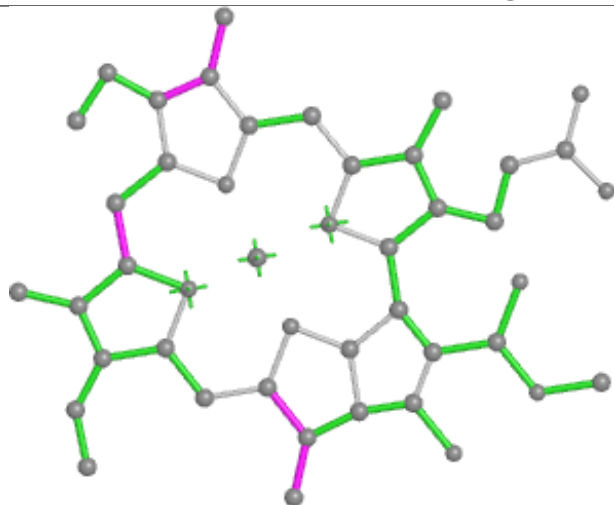


Rings

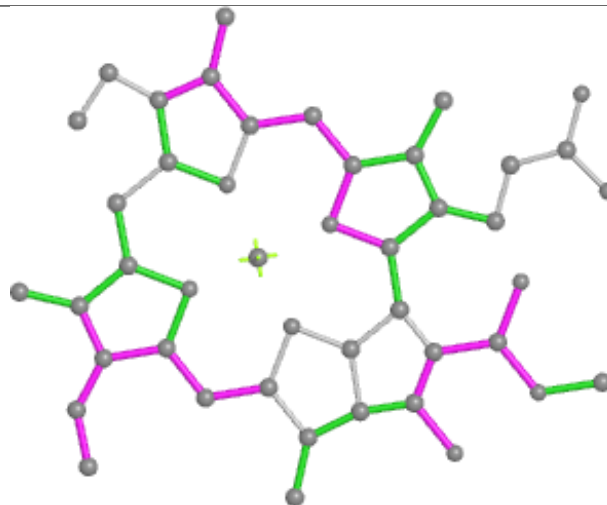
Ligand CLA BB 819



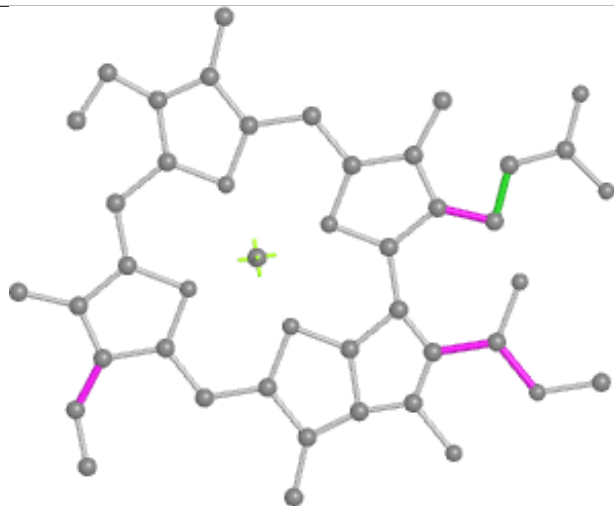
Ligand CLA BB 820



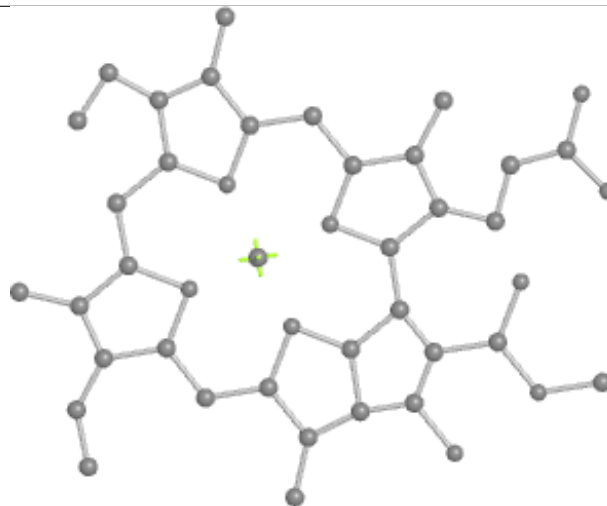
Bond lengths



Bond angles

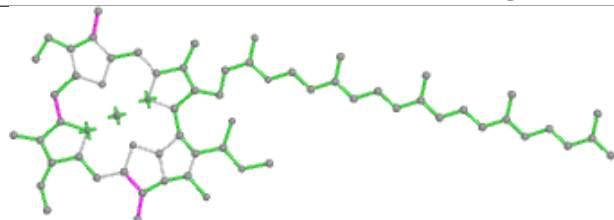


Torsions

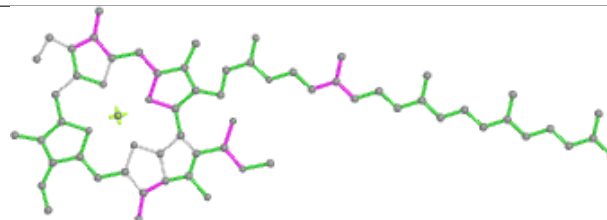


Rings

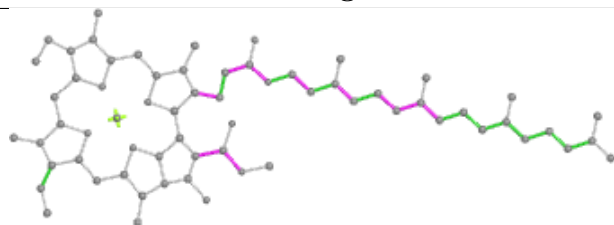
Ligand CLA BB 821



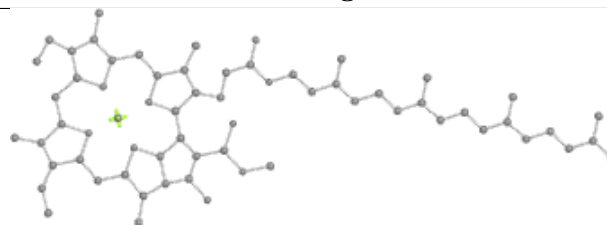
Bond lengths



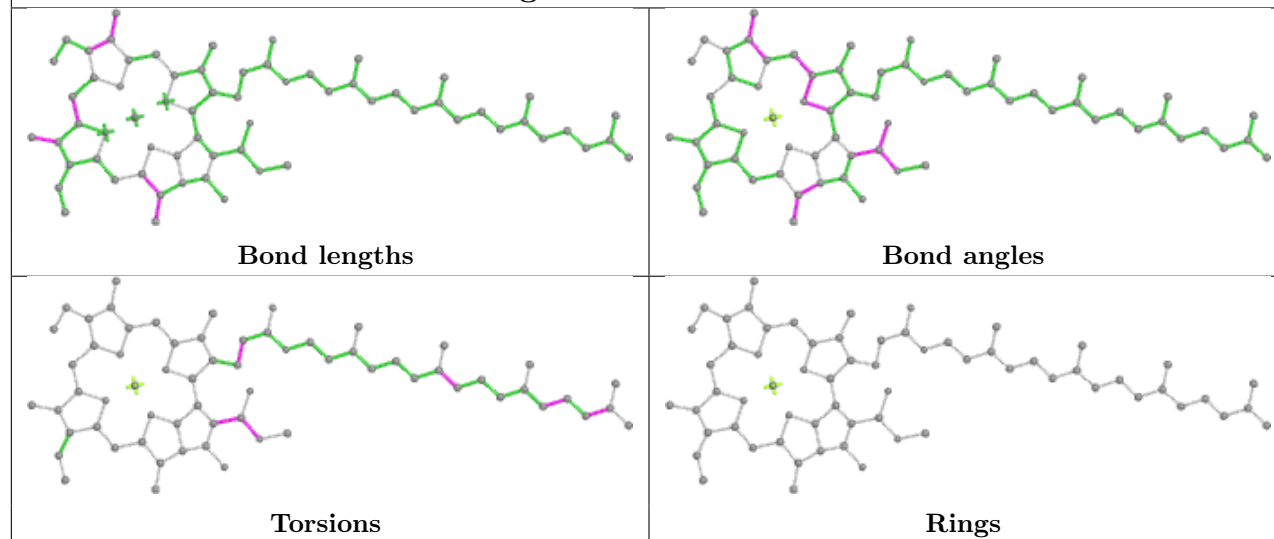
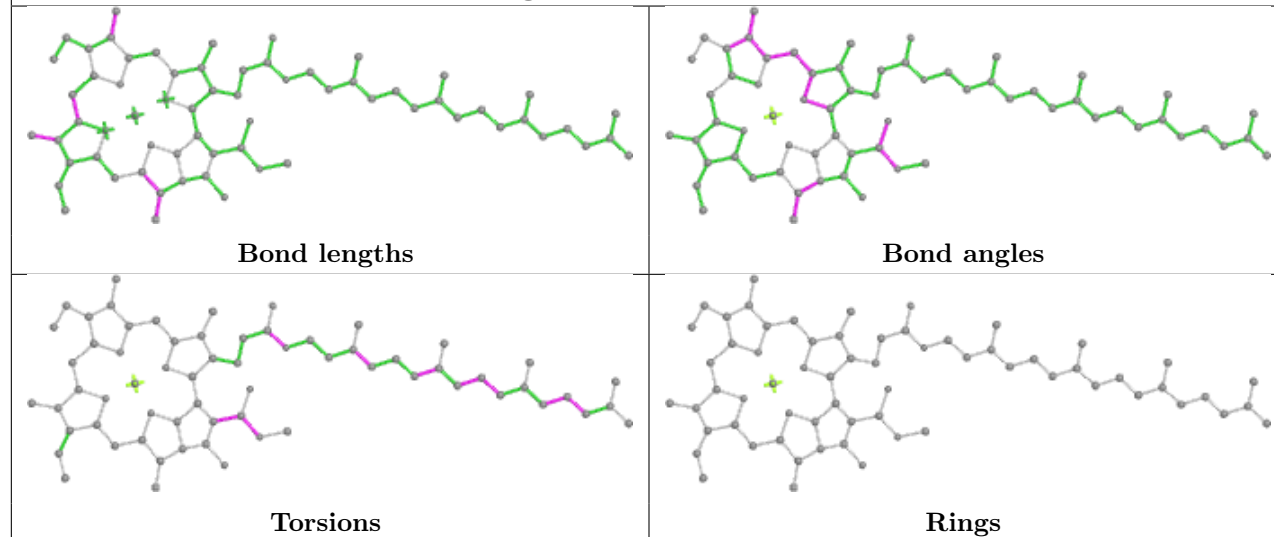
Bond angles



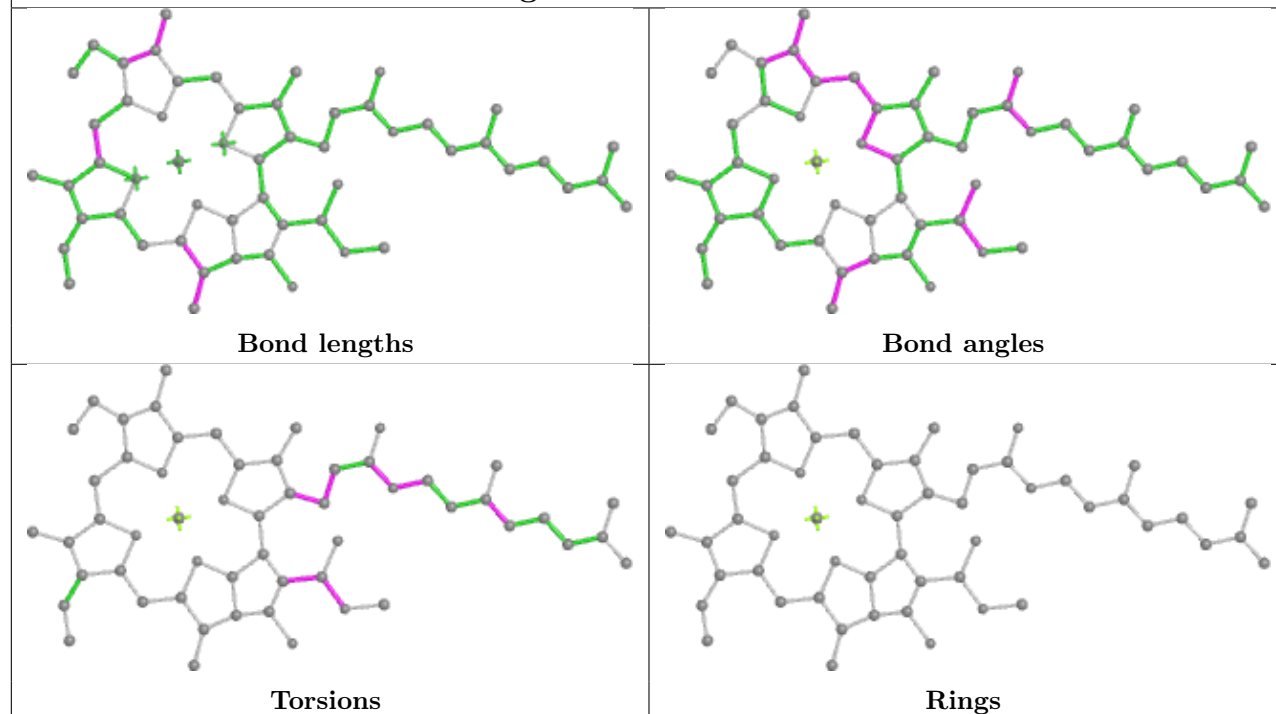
Torsions



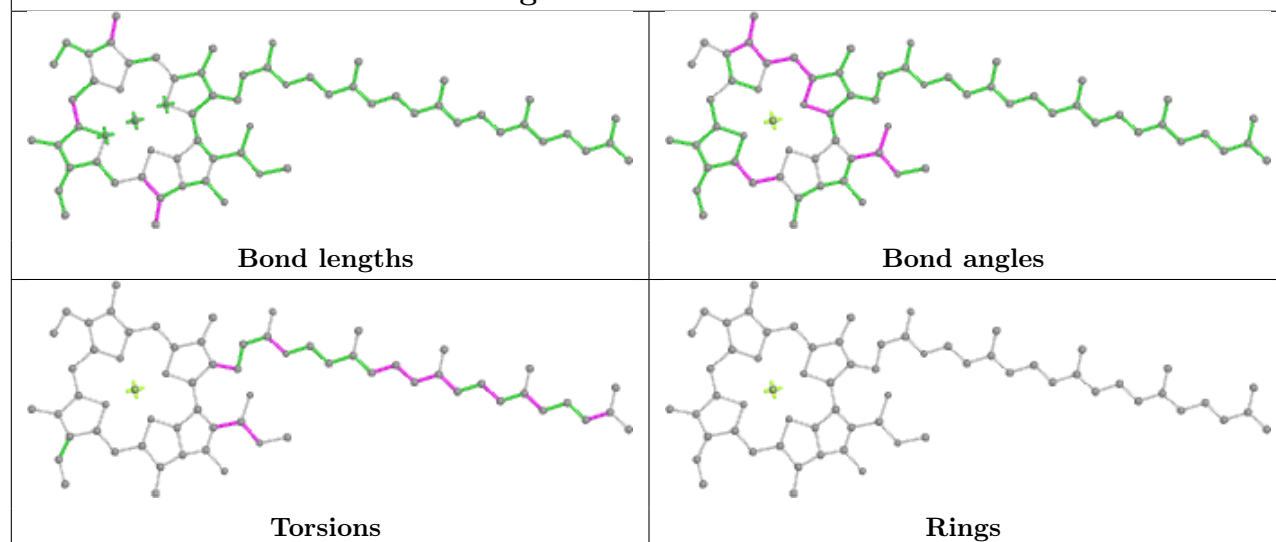
Rings

Ligand CLA BB 822**Ligand CLA BB 823**

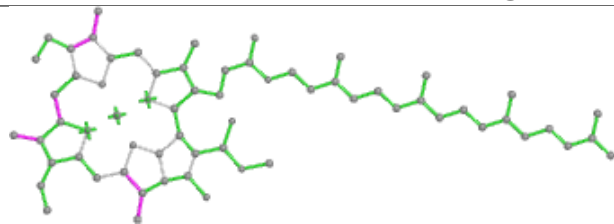
Ligand CLA BB 824



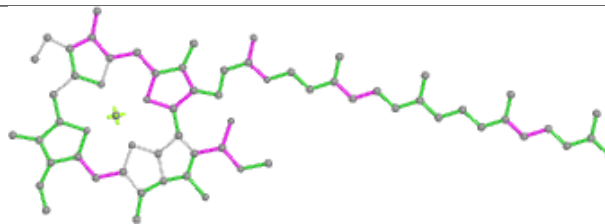
Ligand CLA BB 825



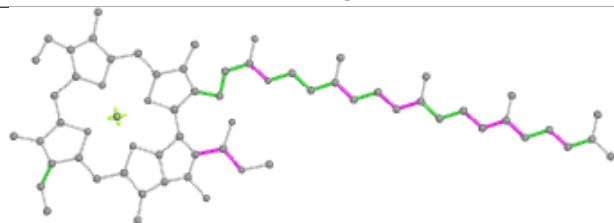
Ligand CLA BB 826



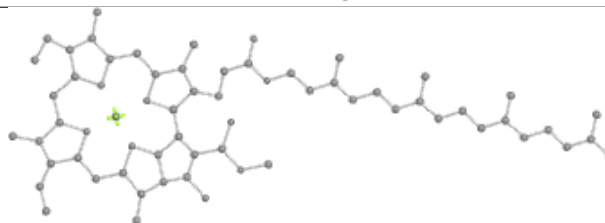
Bond lengths



Bond angles

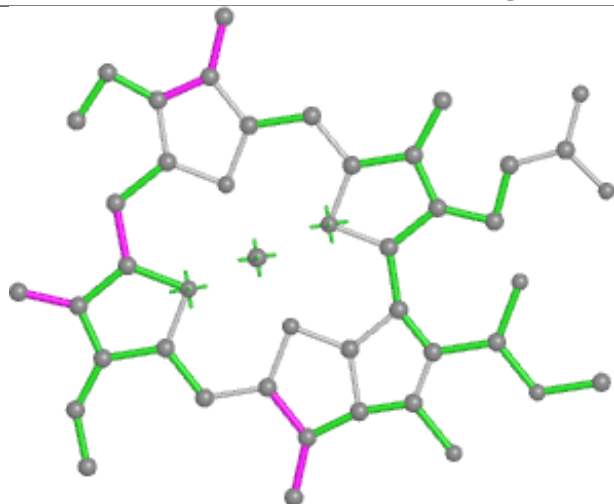


Torsions

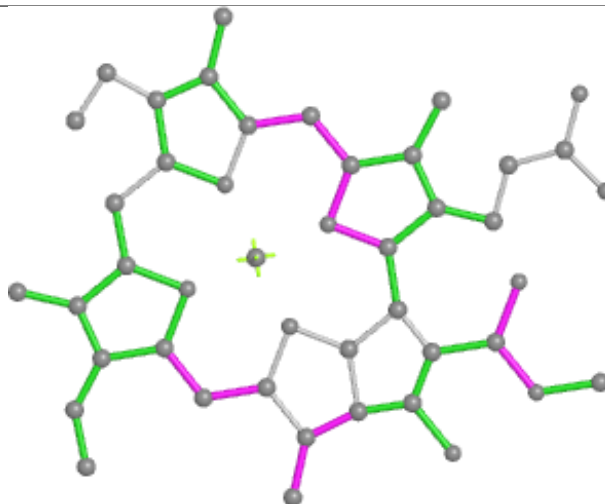


Rings

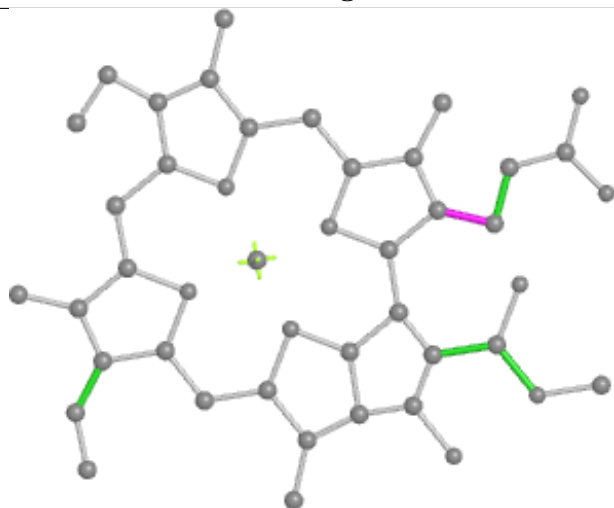
Ligand CLA BB 827



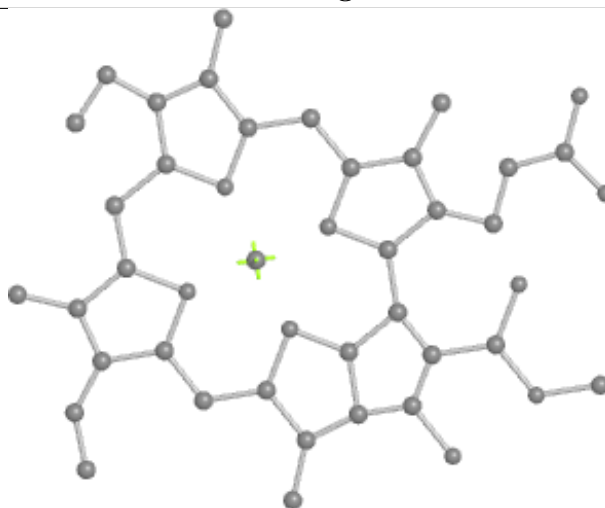
Bond lengths



Bond angles

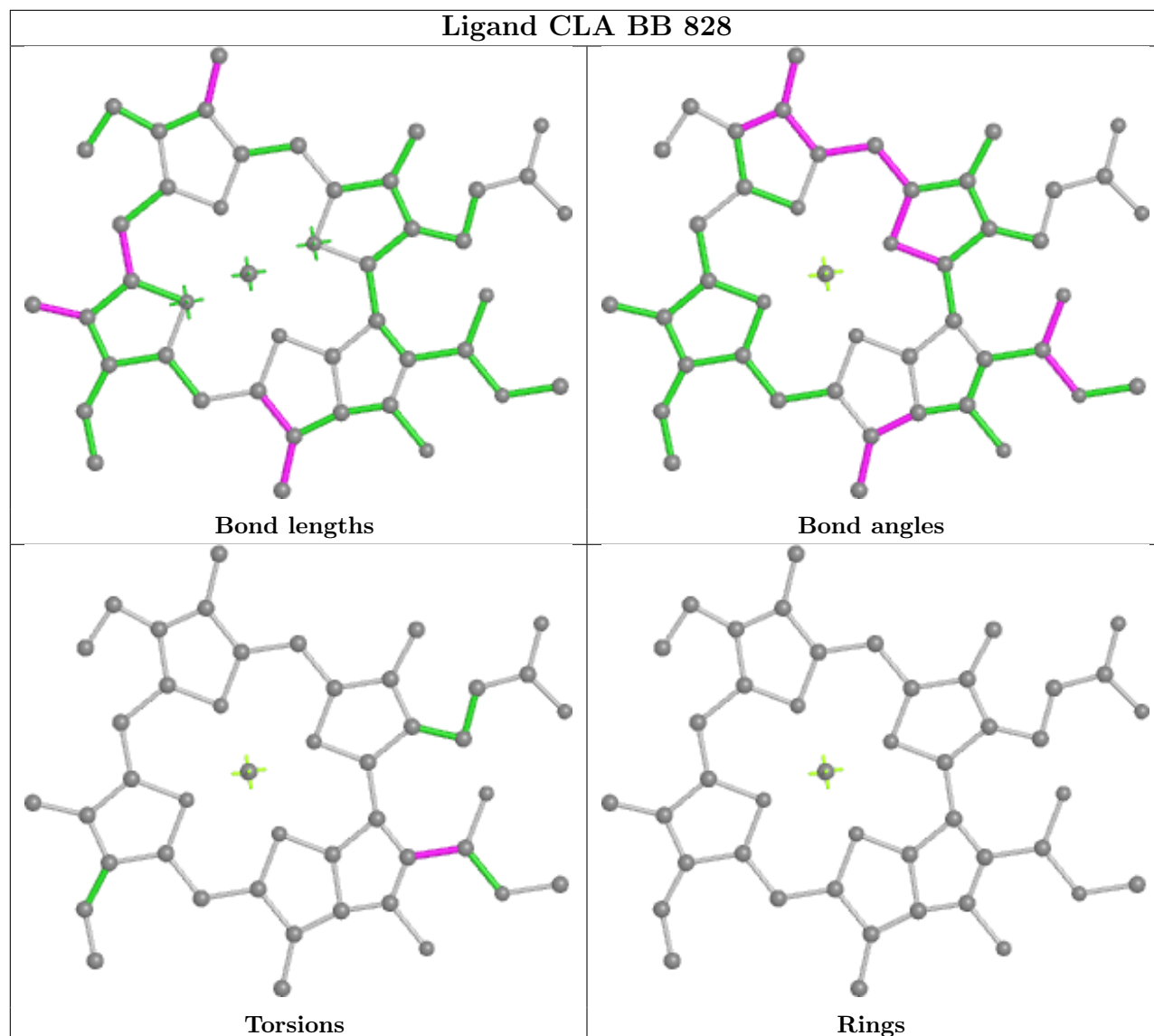


Torsions

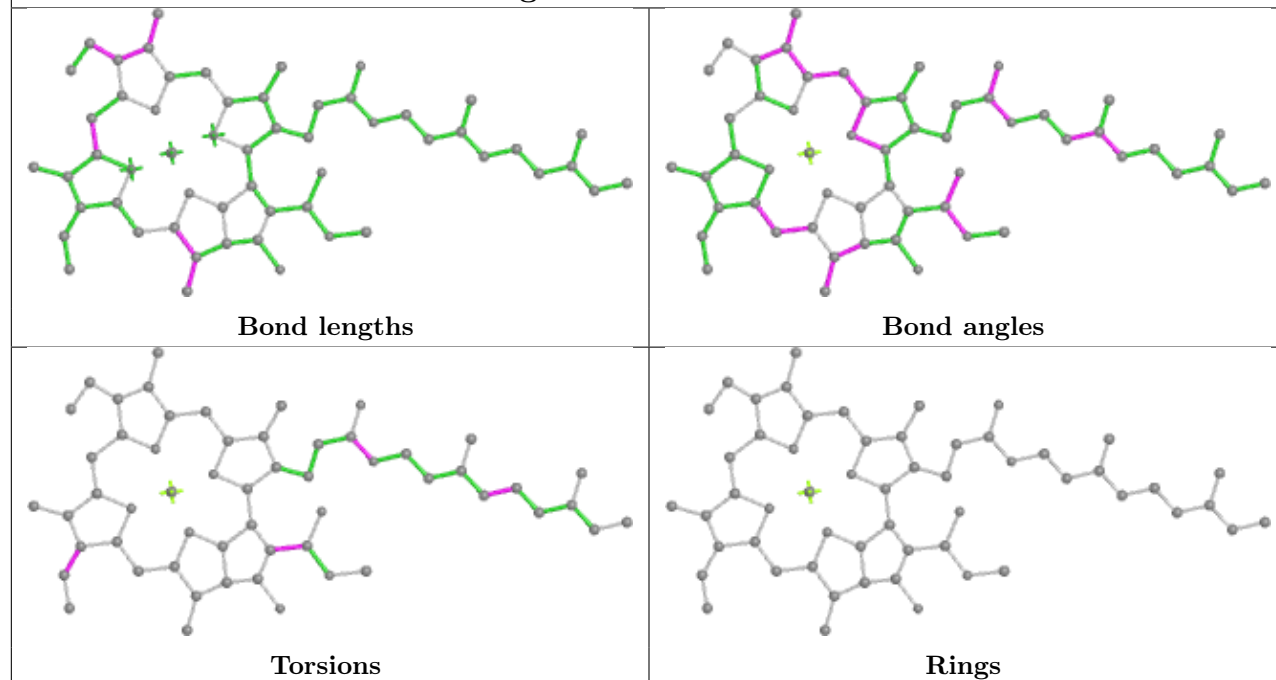


Rings

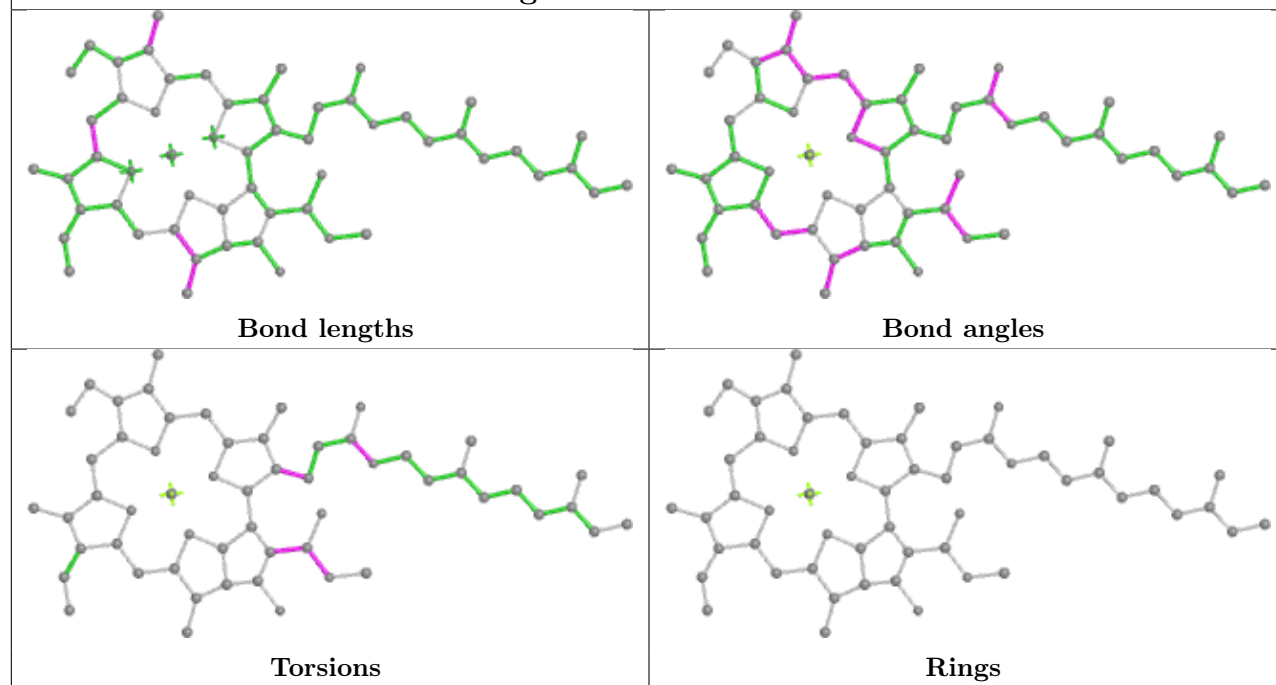
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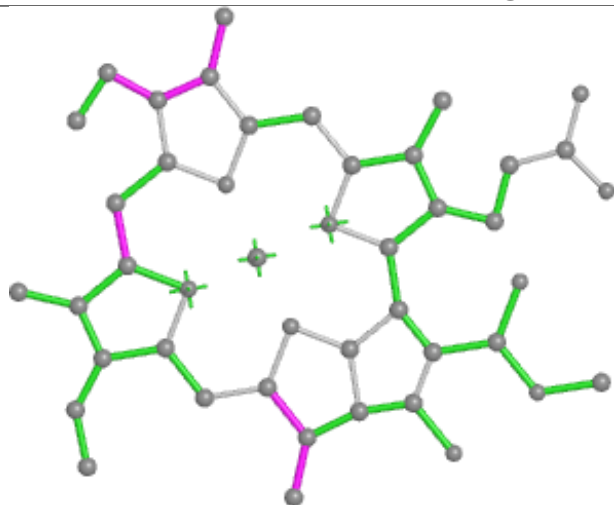
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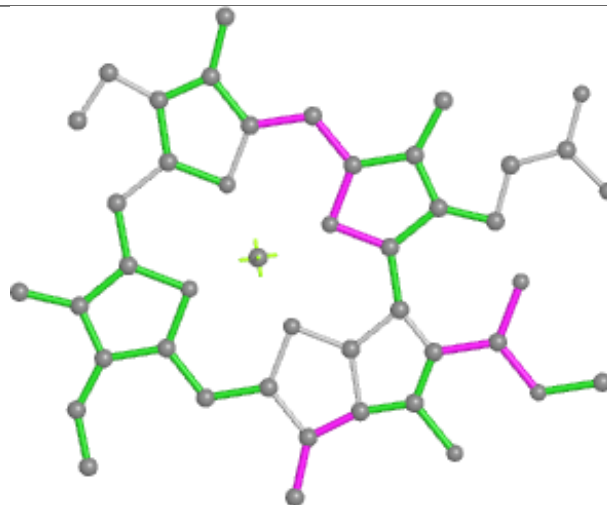
Ligand CLA BB 830



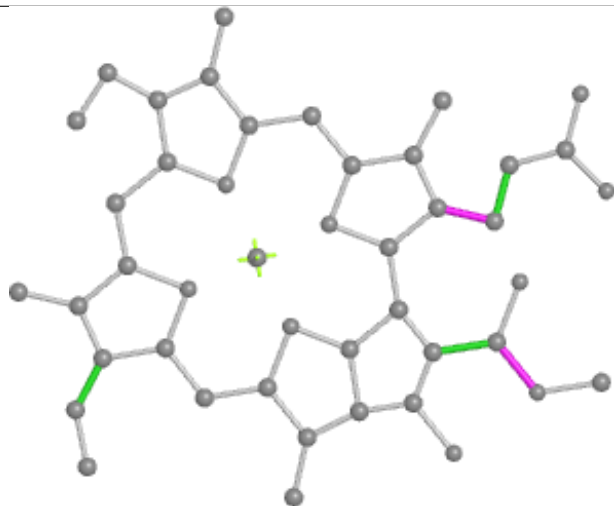
Ligand CLA BB 831



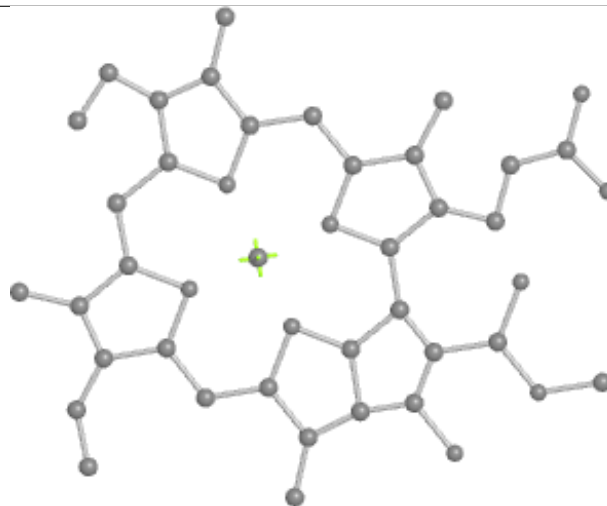
Bond lengths



Bond angles

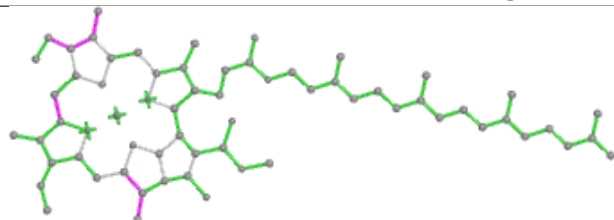


Torsions

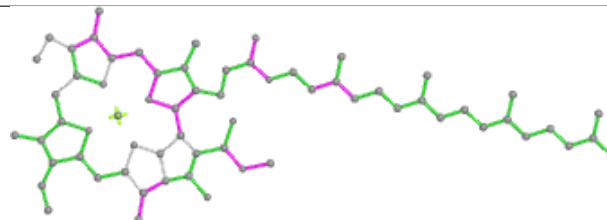


Rings

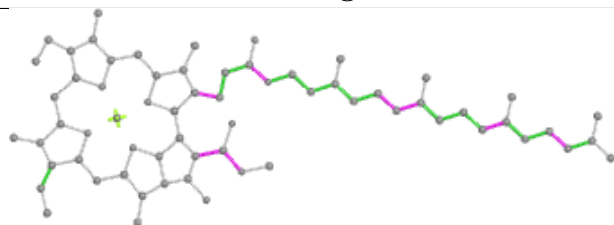
Ligand CLA BB 832



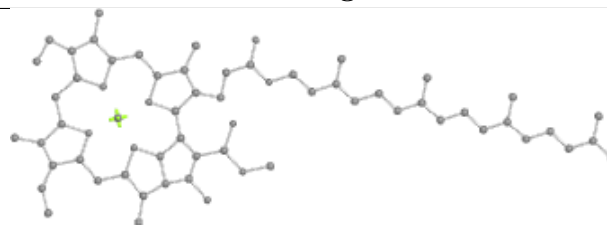
Bond lengths



Bond angles

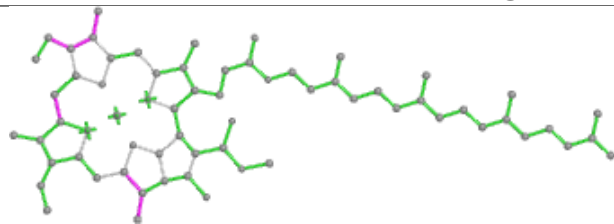


Torsions

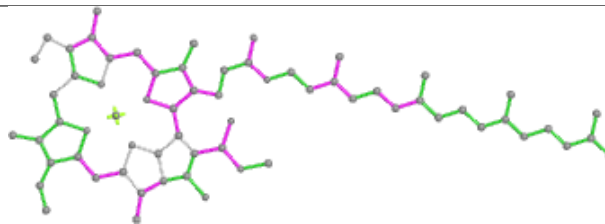


Rings

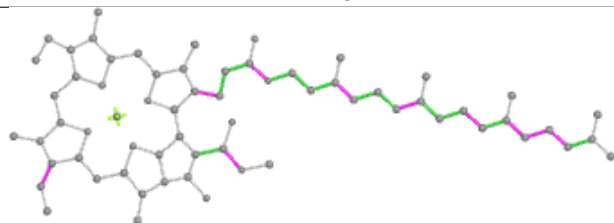
Ligand CLA BB 833



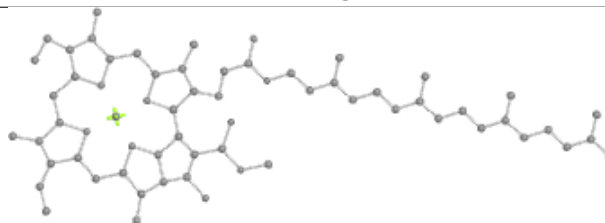
Bond lengths



Bond angles

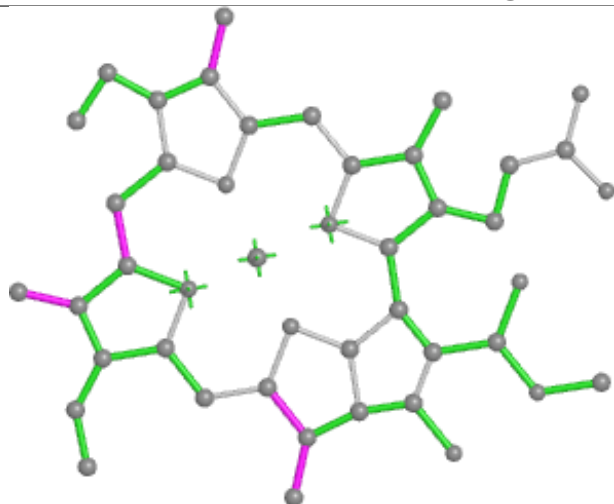


Torsions

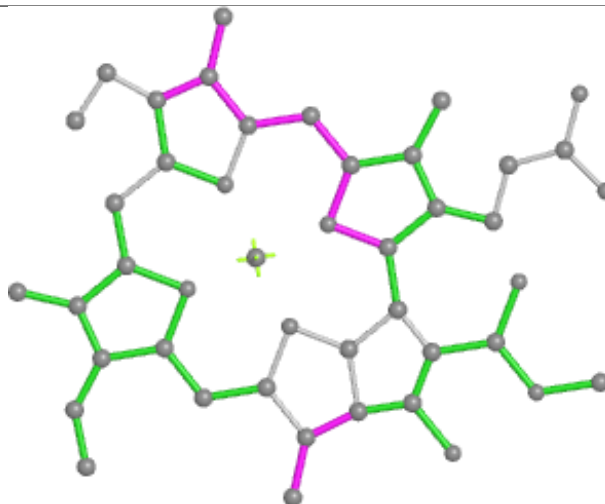


Rings

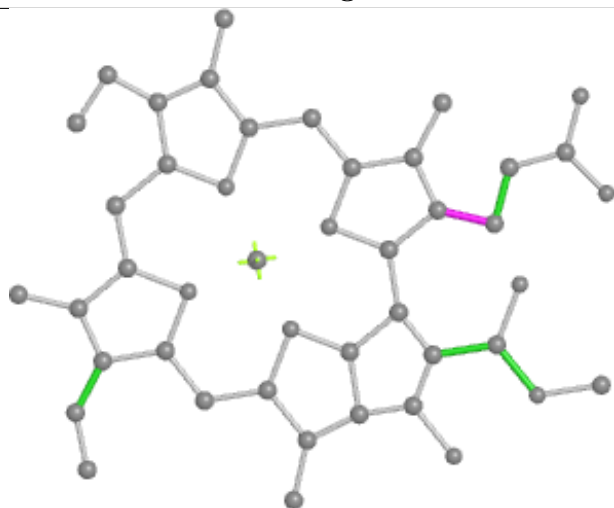
Ligand CLA BB 834



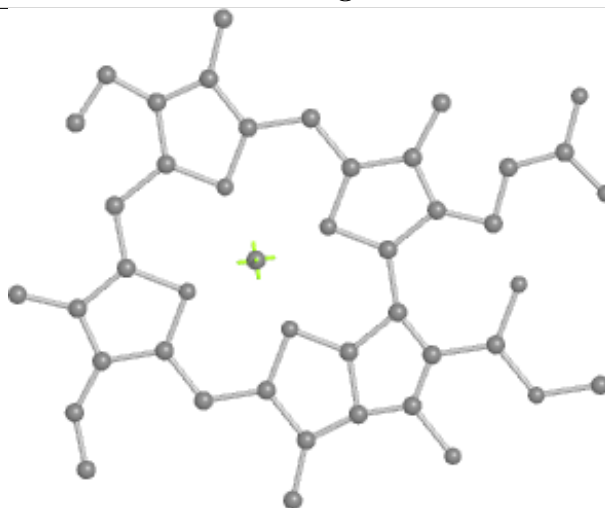
Bond lengths



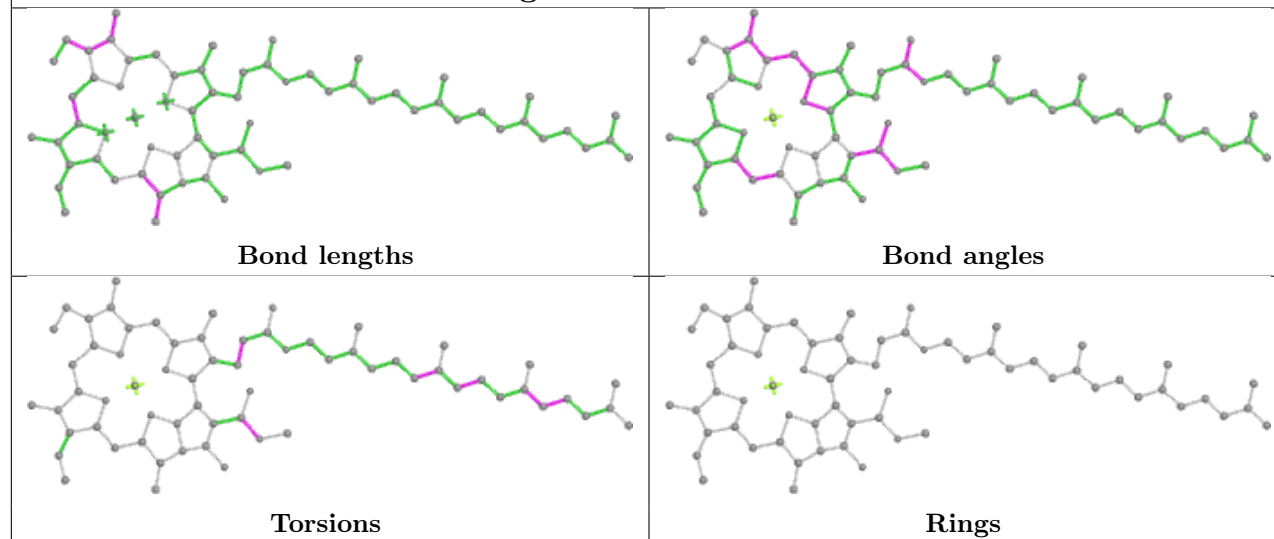
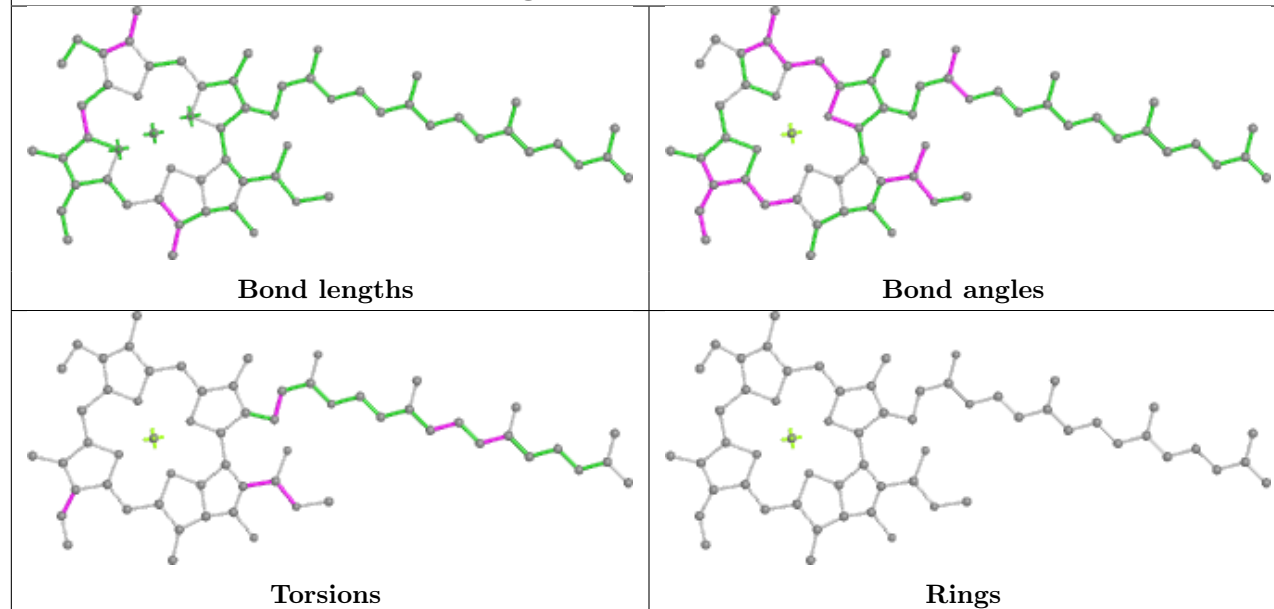
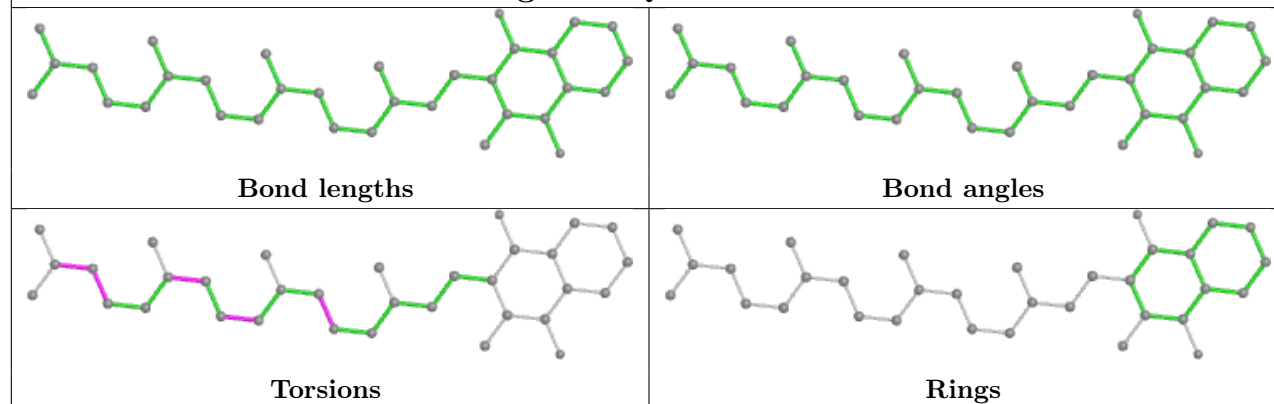
Bond angles

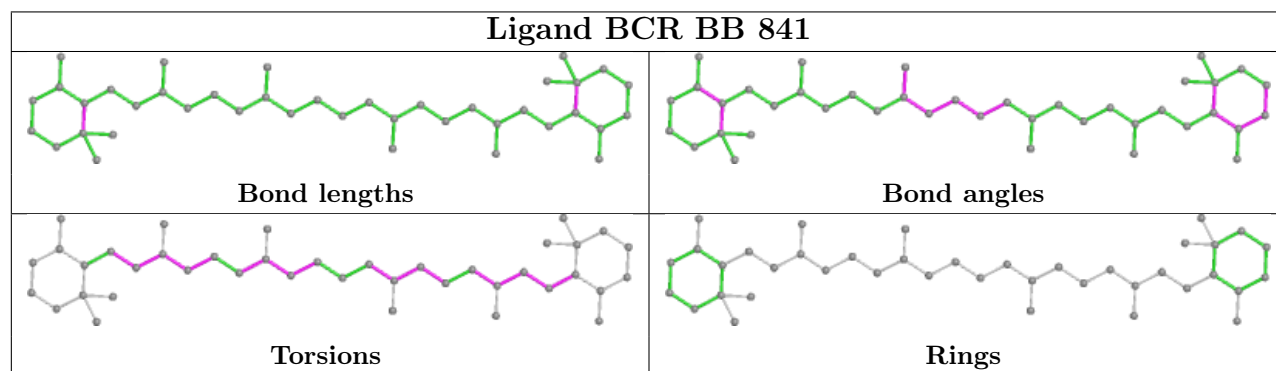
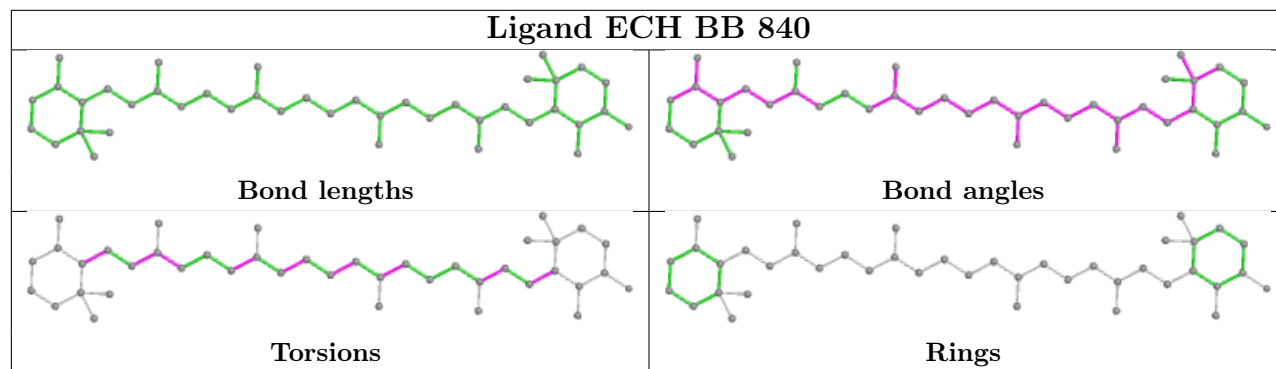
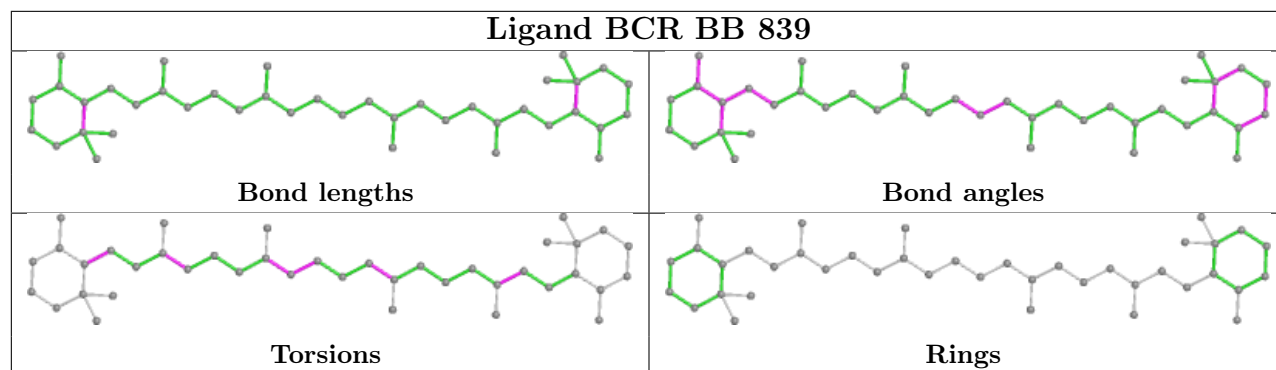
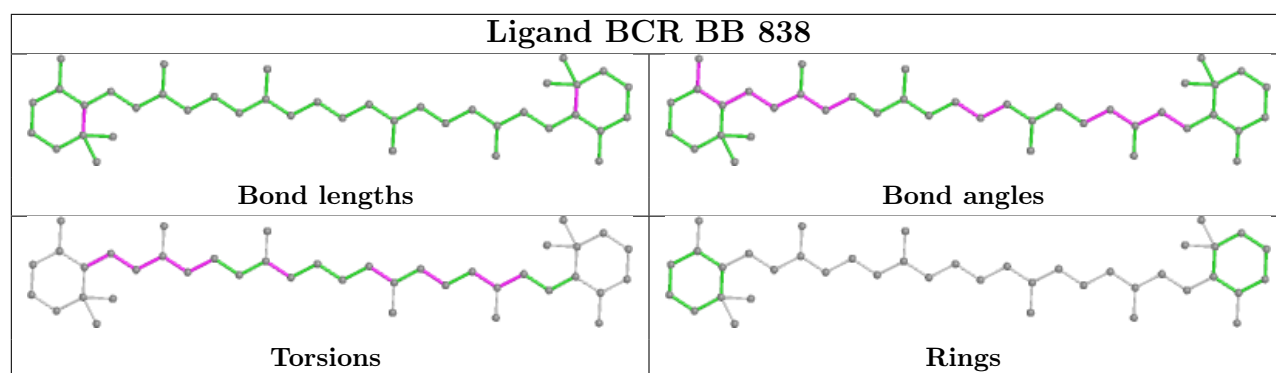


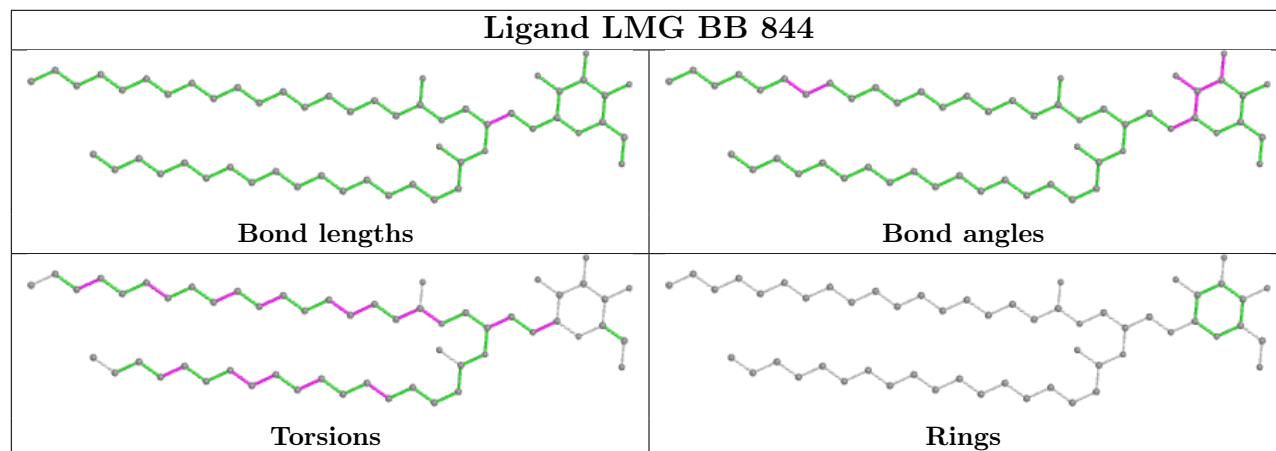
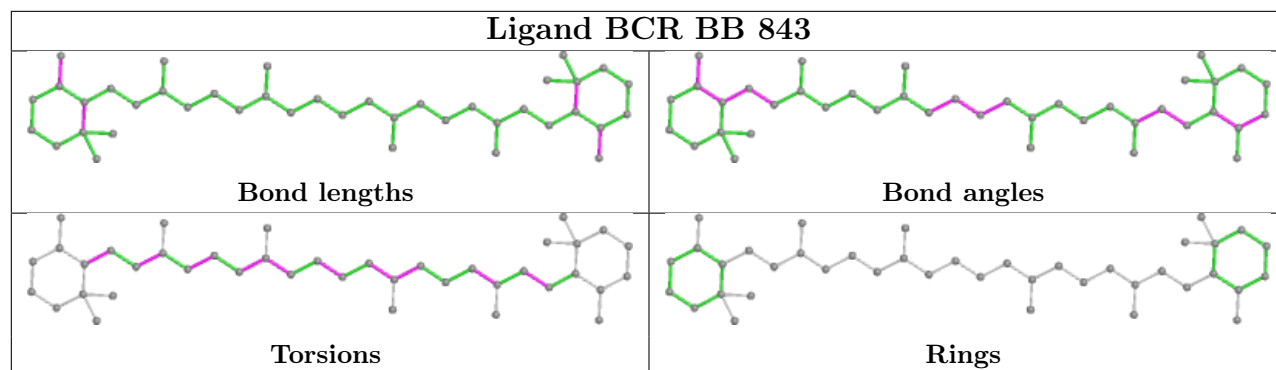
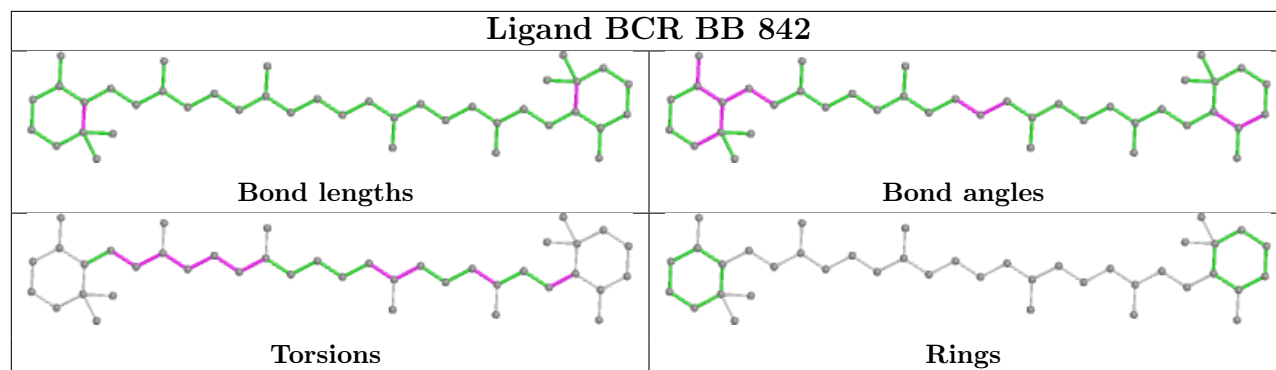
Torsions



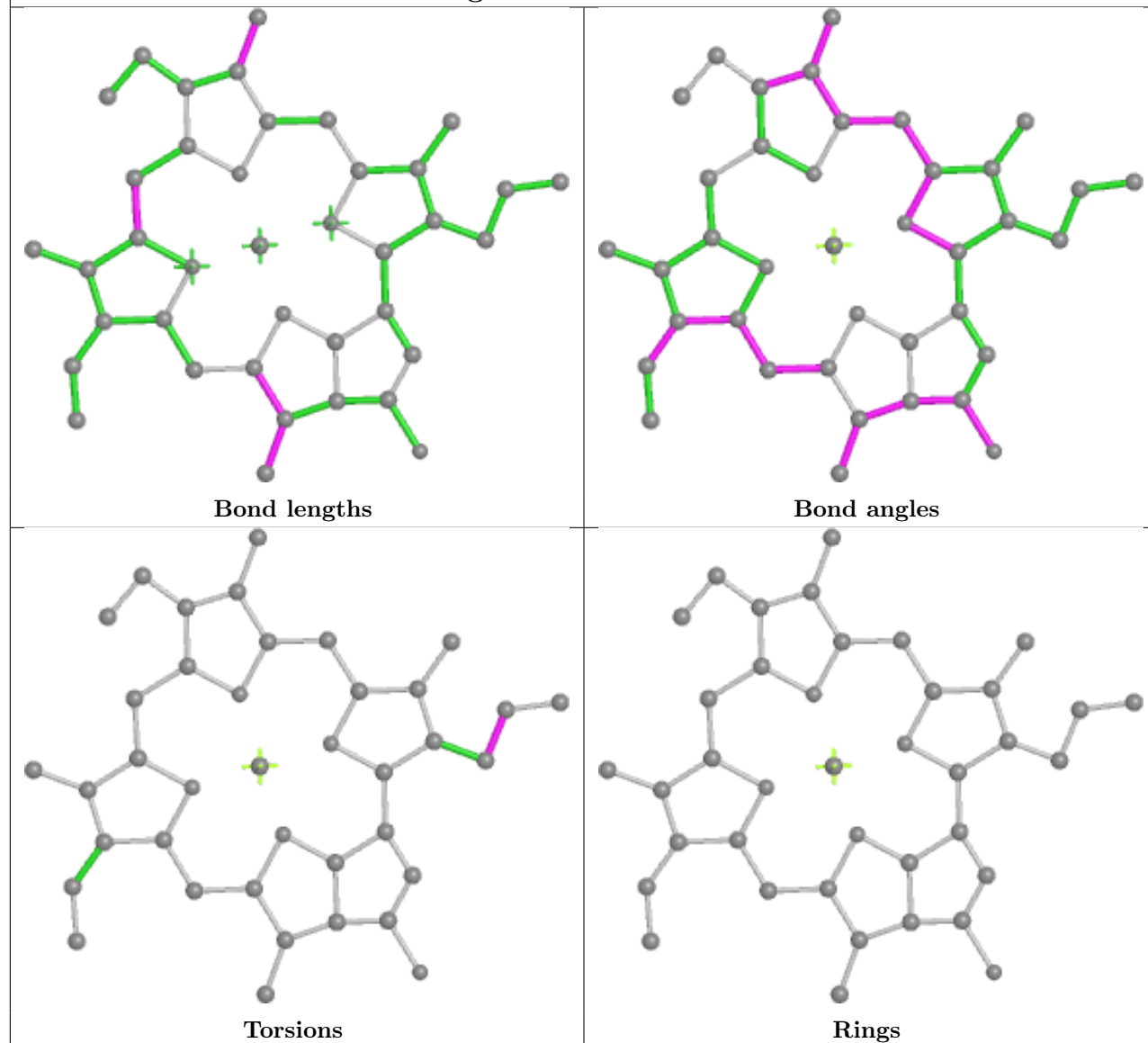
Rings

Ligand CLA BB 835**Ligand CLA BB 836****Ligand PQN BB 837**

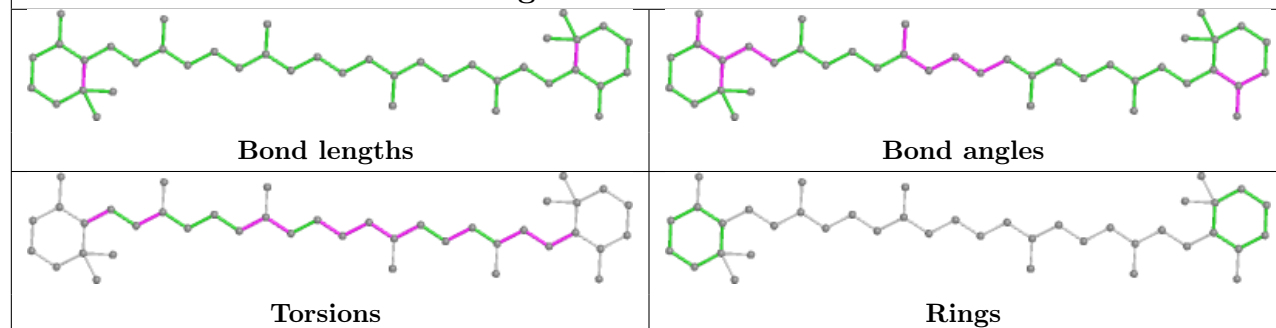


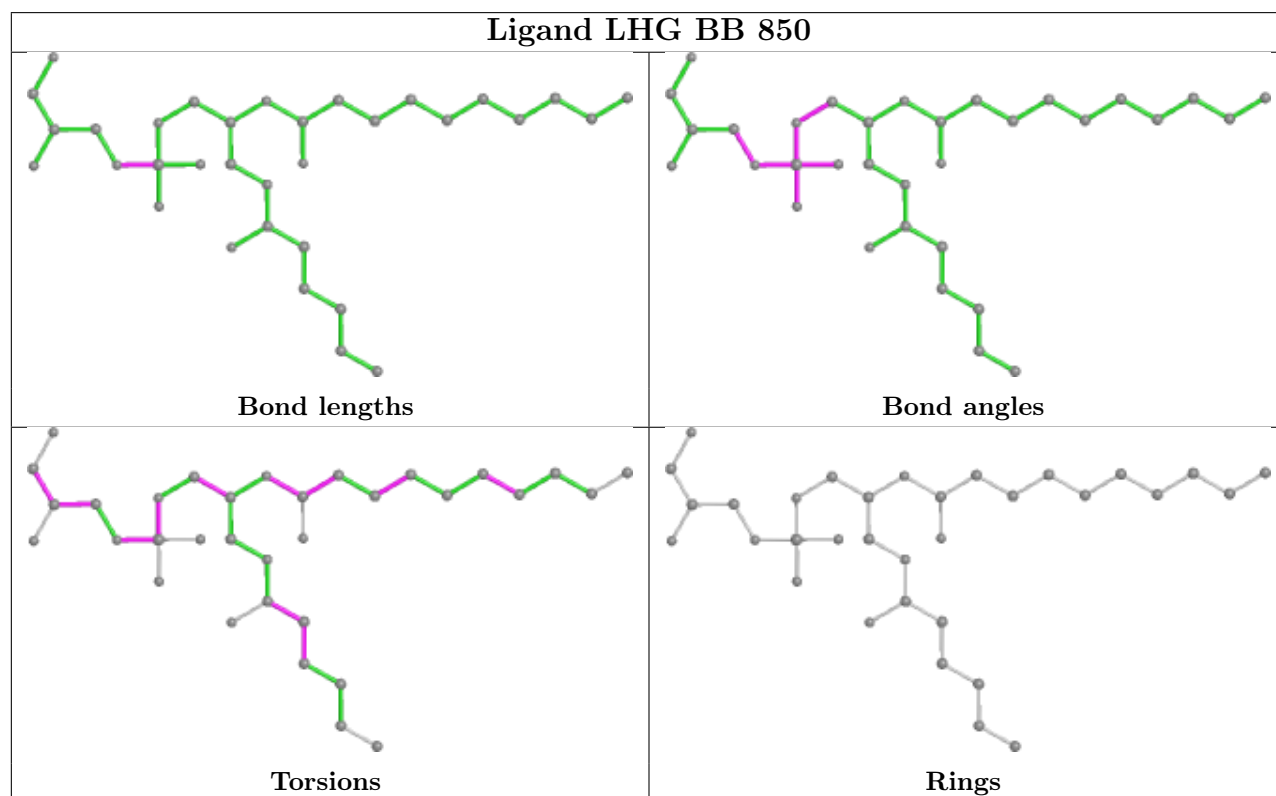
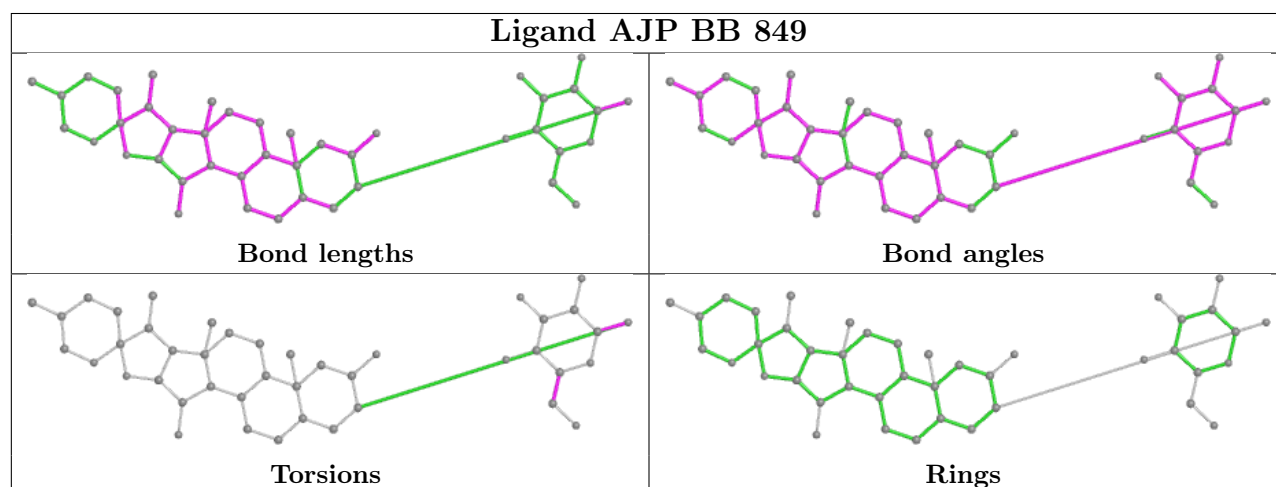
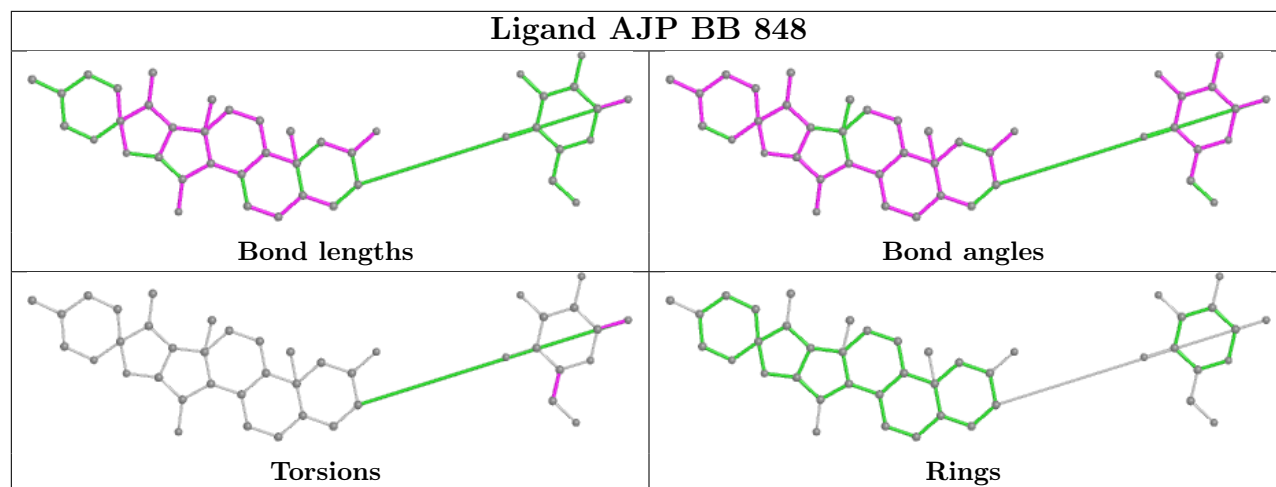


Ligand CLA BB 845

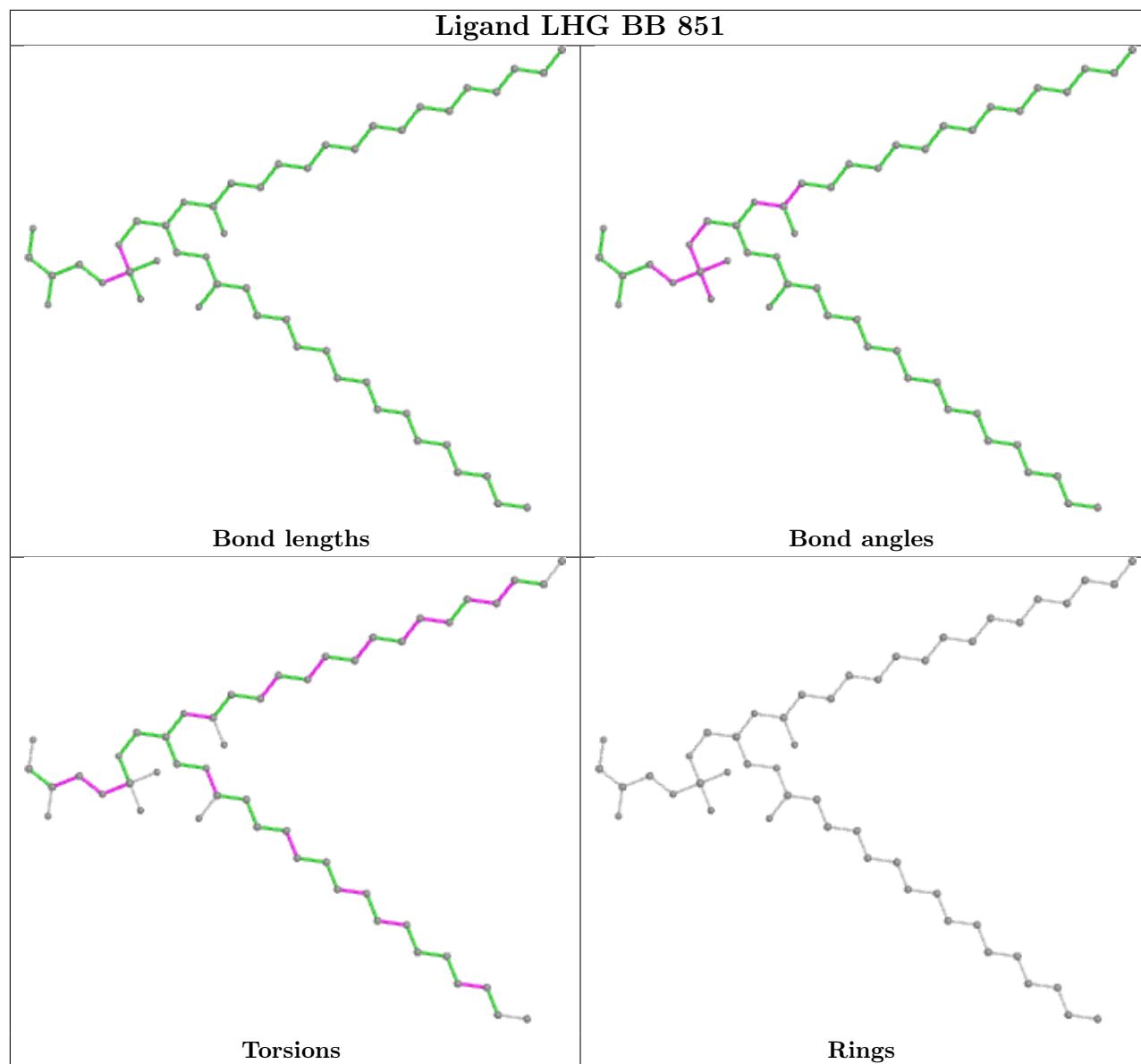


Ligand BCR BB 847

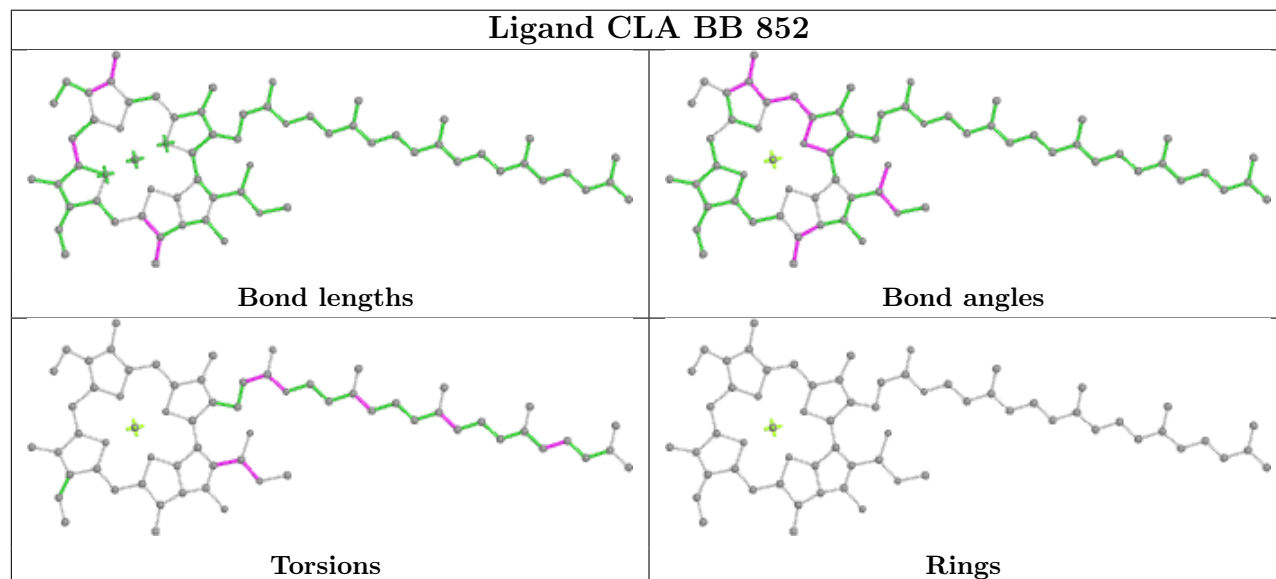




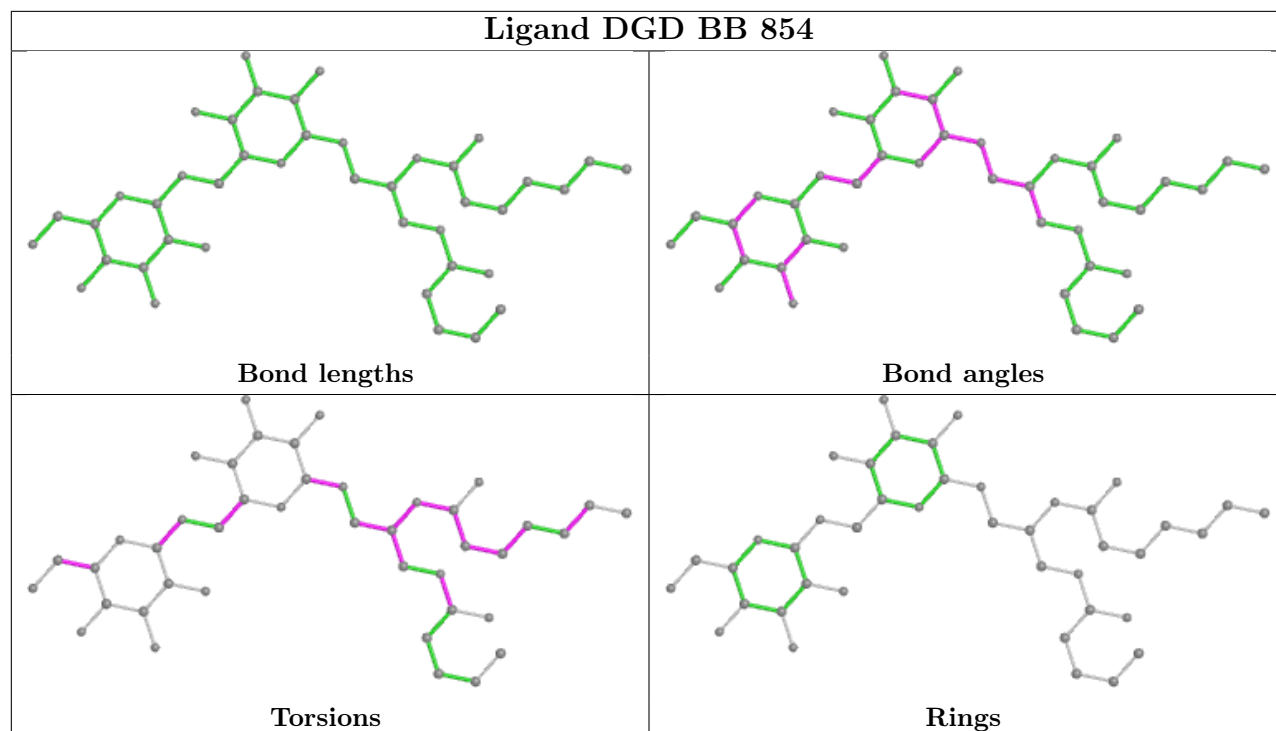
Ligand LHG BB 851



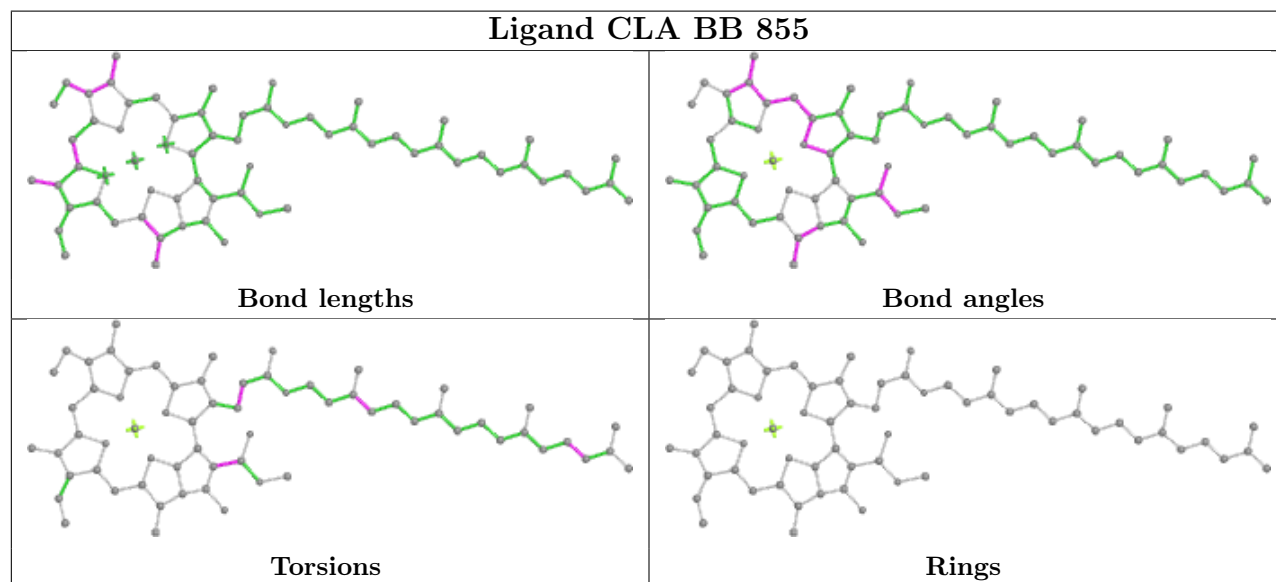
Ligand CLA BB 852

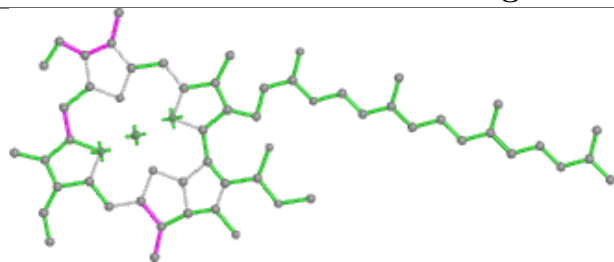


Ligand DGD BB 854

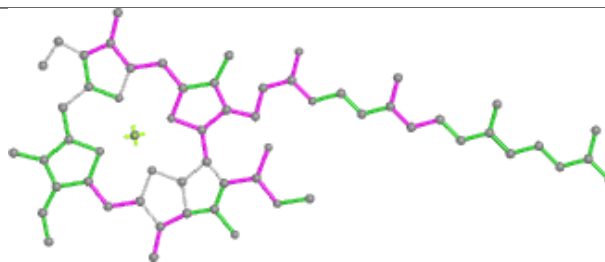


Ligand CLA BB 855

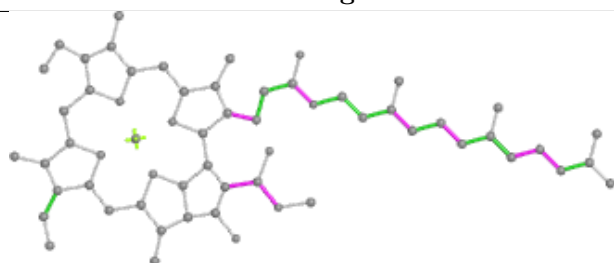


Ligand CLA BB 856

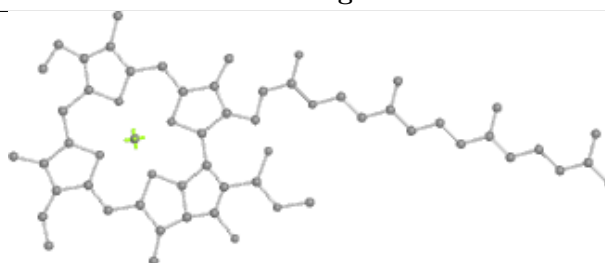
Bond lengths



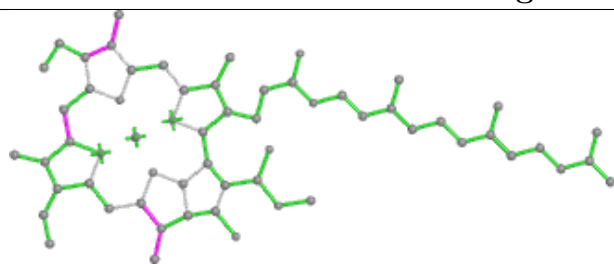
Bond angles



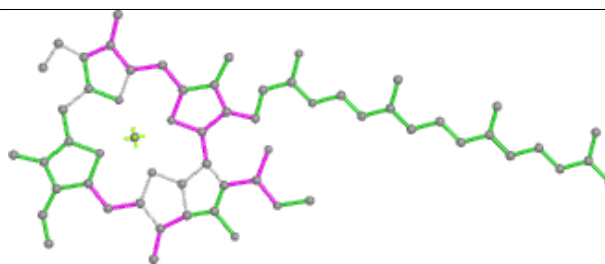
Torsions



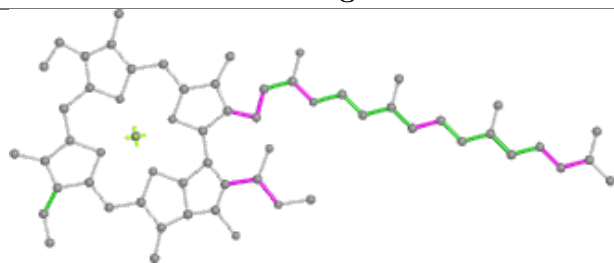
Rings

Ligand CLA F 301

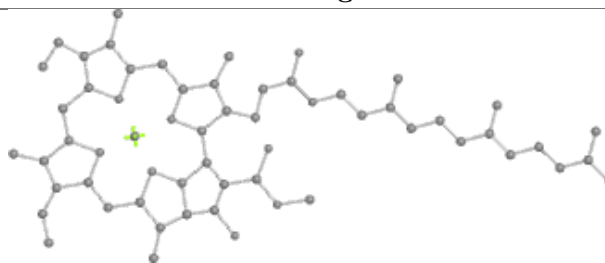
Bond lengths



Bond angles

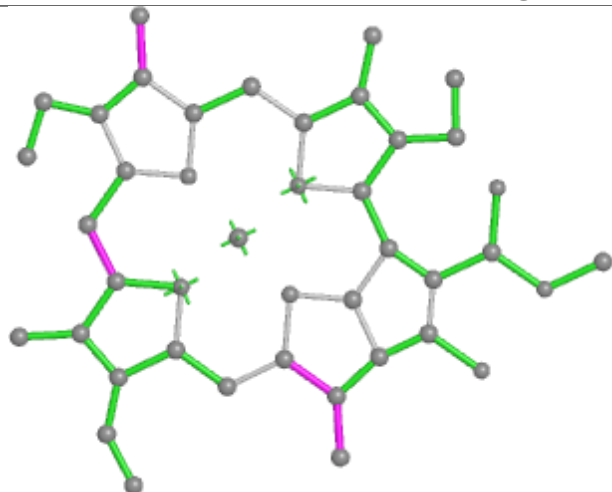


Torsions

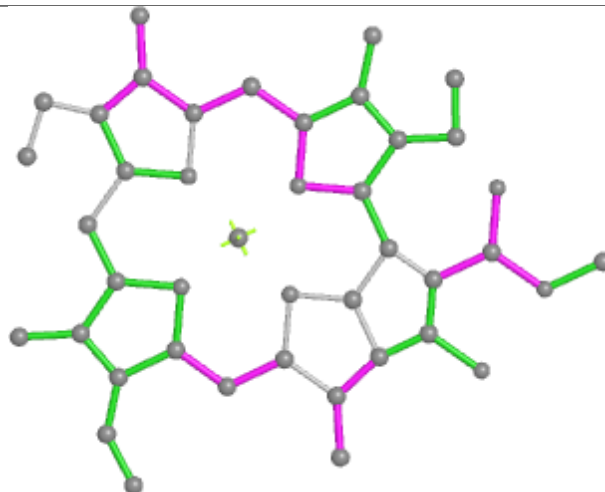


Rings

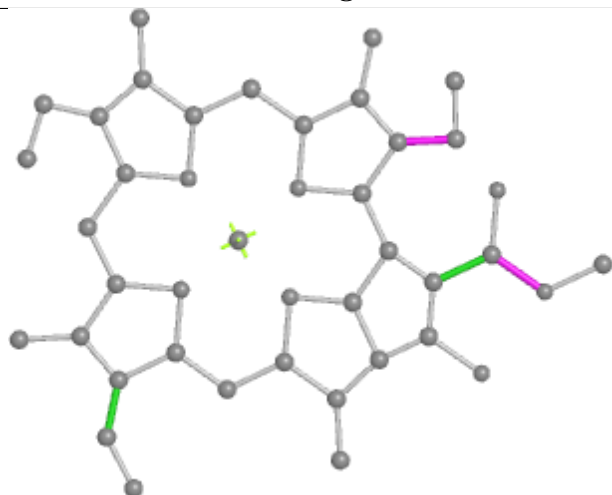
Ligand CLA F 302



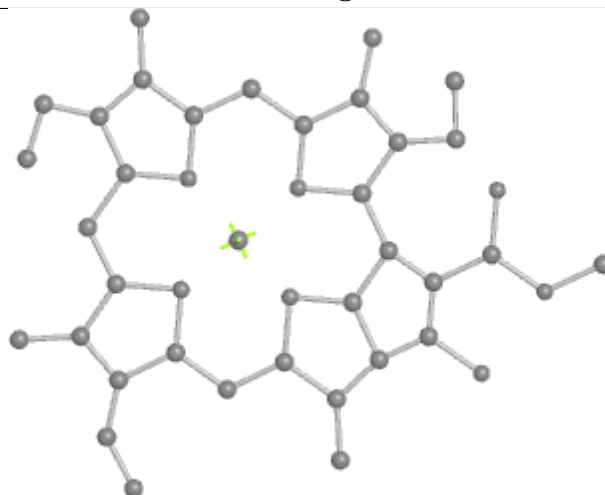
Bond lengths



Bond angles

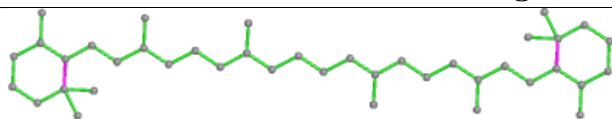


Torsions

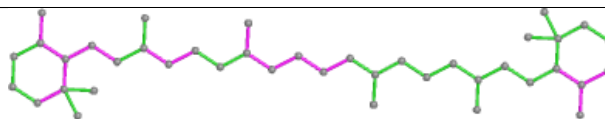


Rings

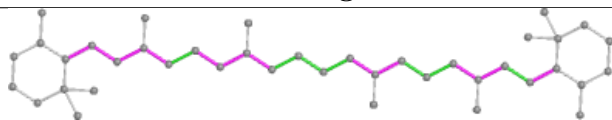
Ligand BCR F 303



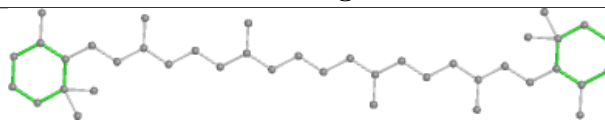
Bond lengths



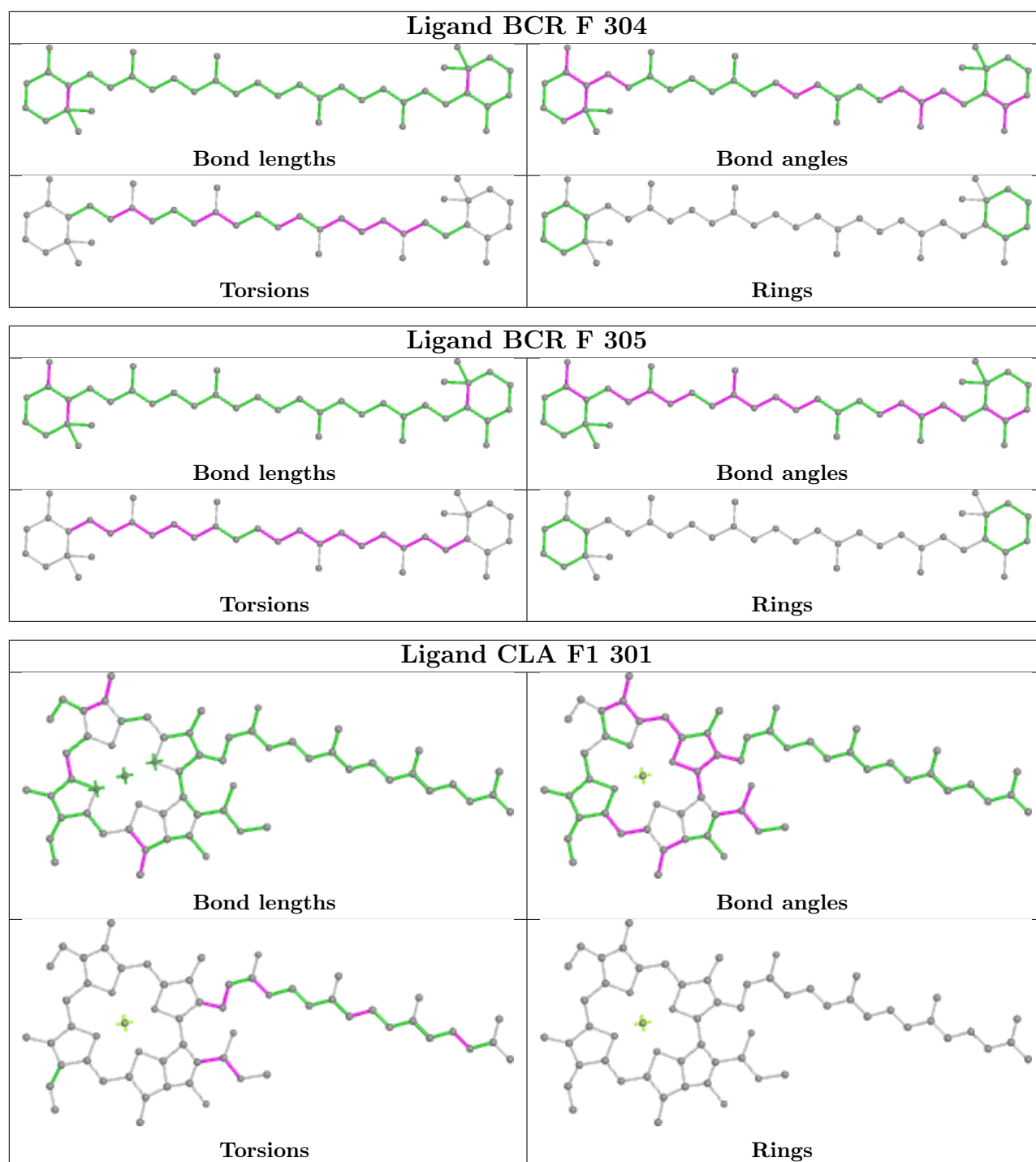
Bond angles



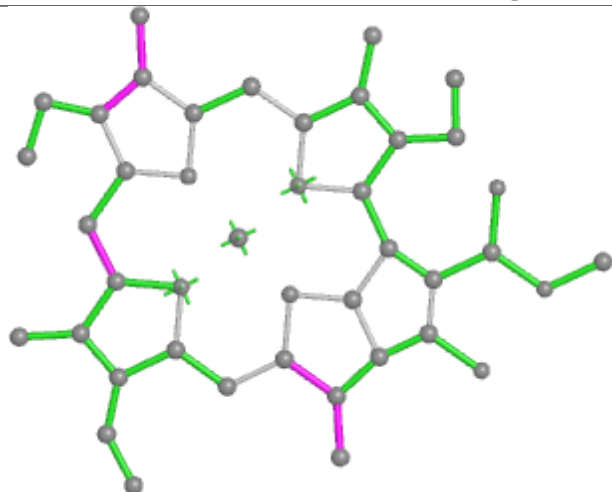
Torsions



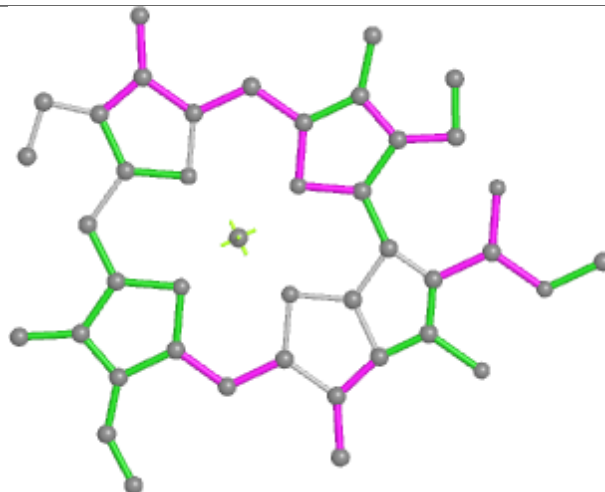
Rings



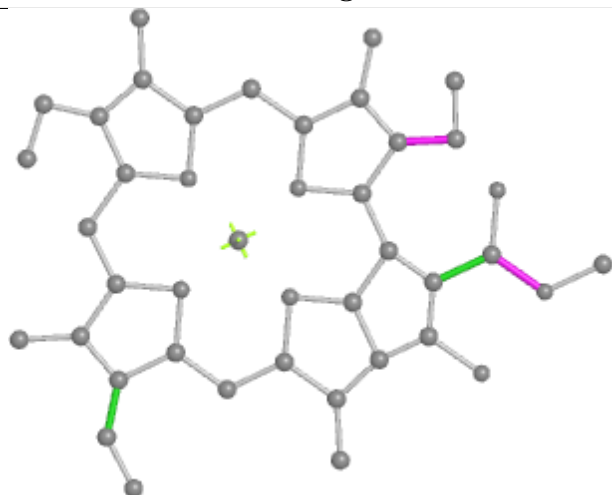
Ligand CLA F1 302



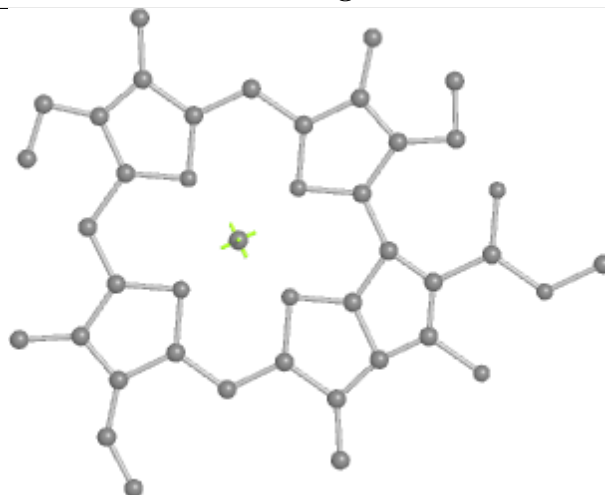
Bond lengths



Bond angles

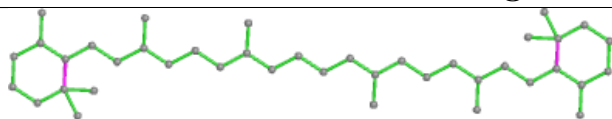


Torsions

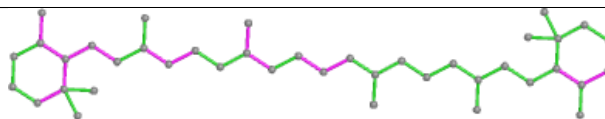


Rings

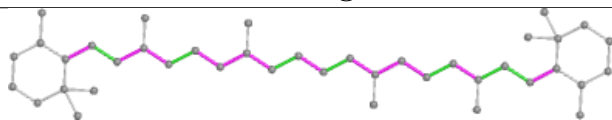
Ligand BCR F1 303



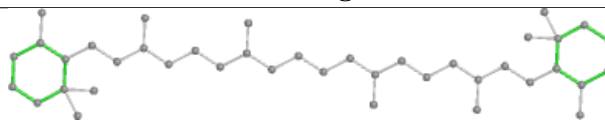
Bond lengths



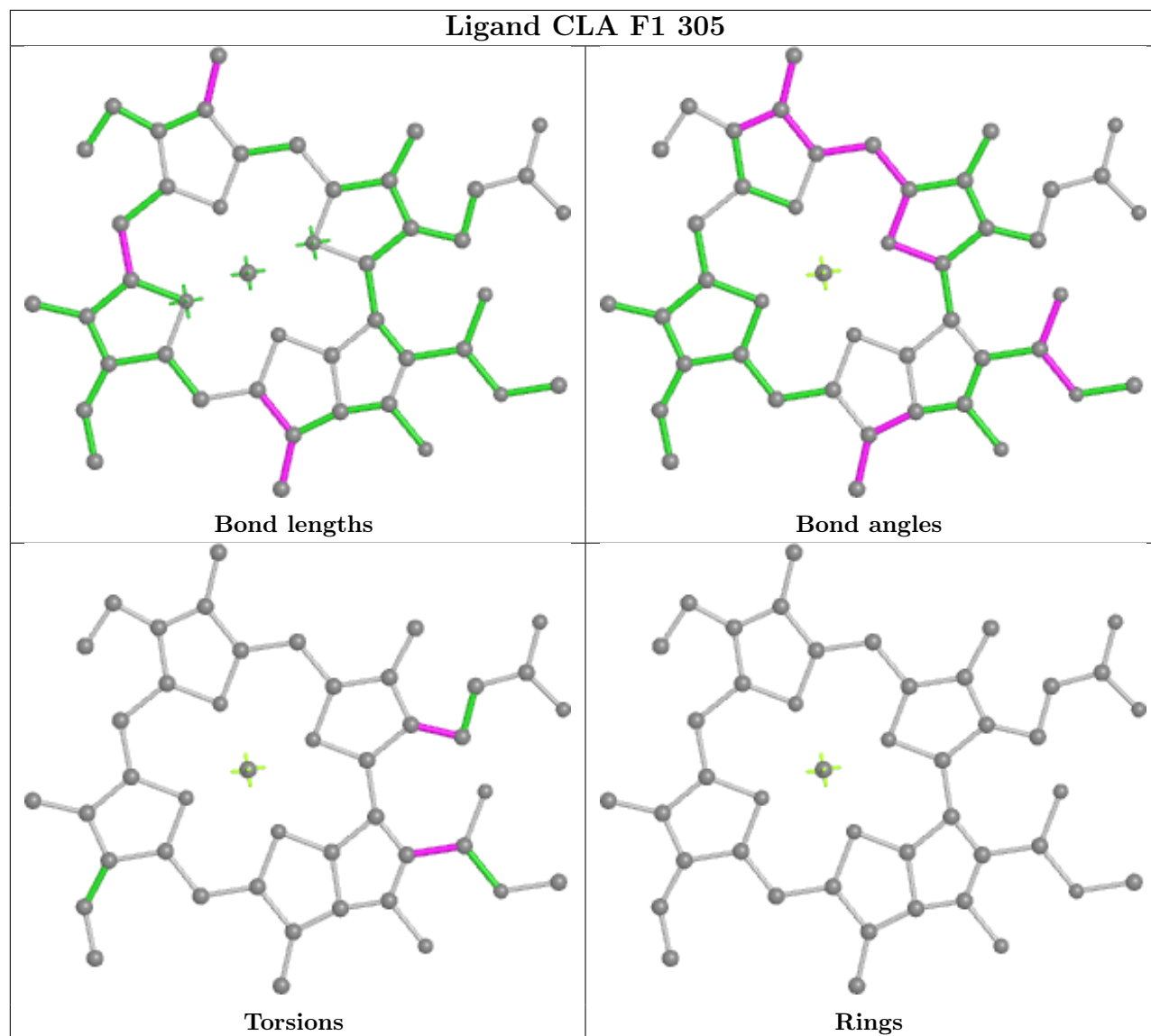
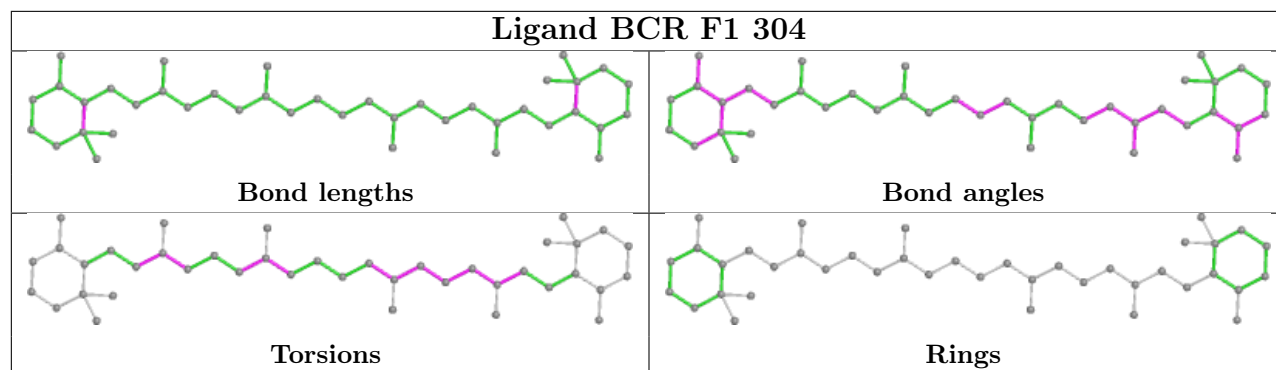
Bond angles

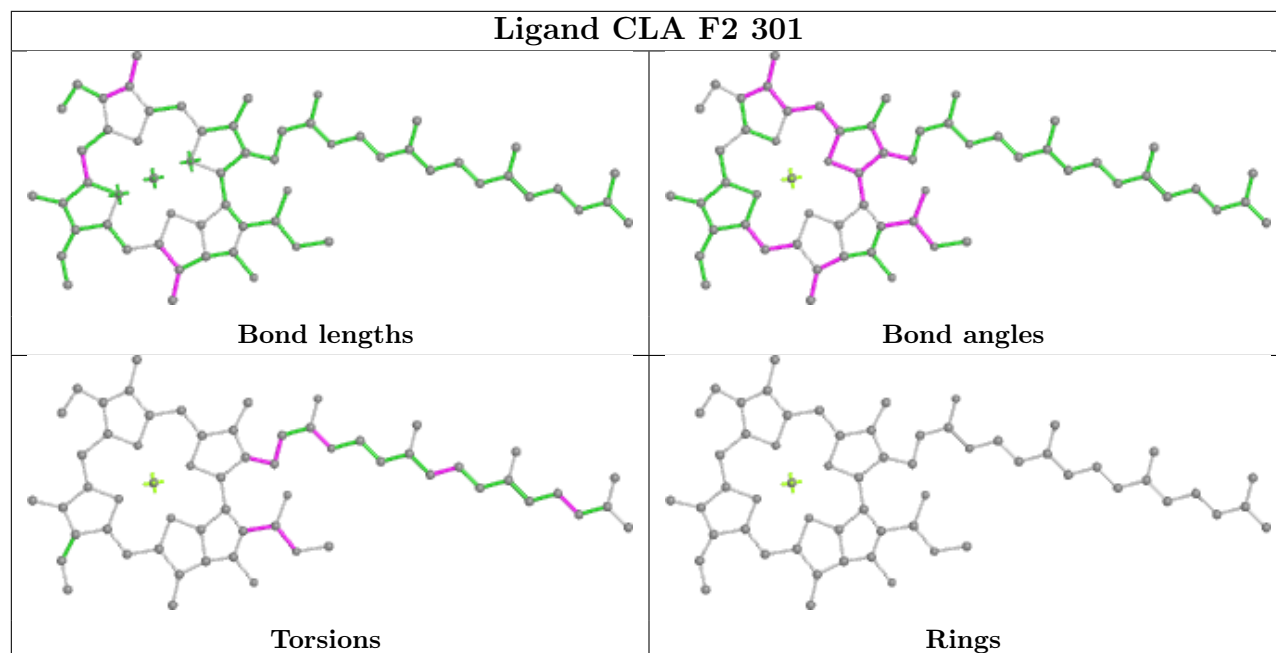
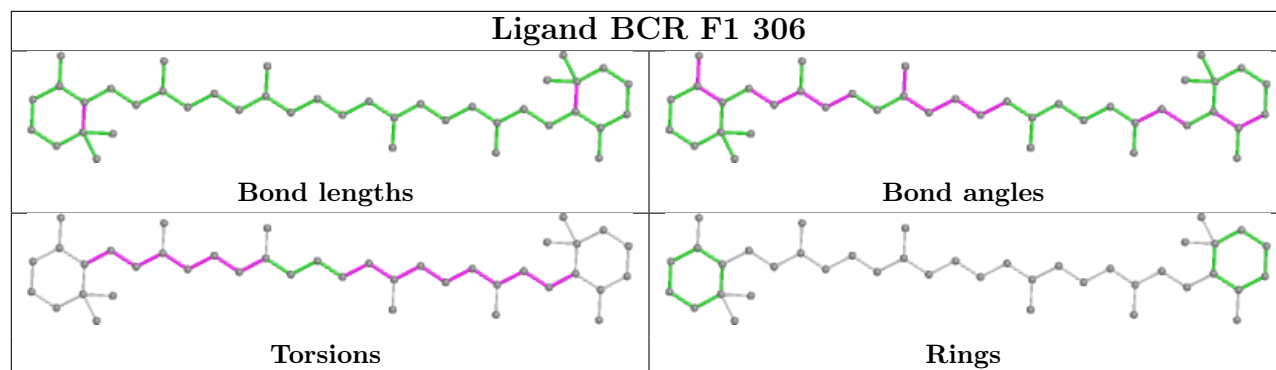


Torsions

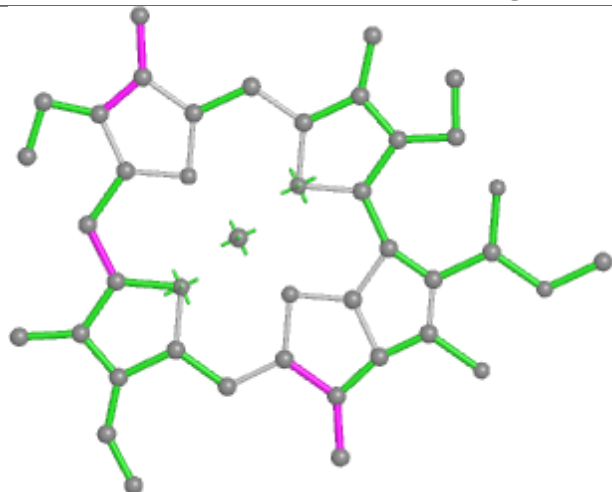


Rings

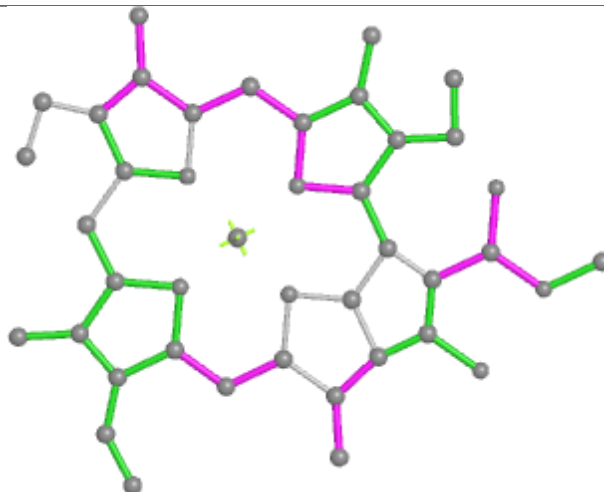




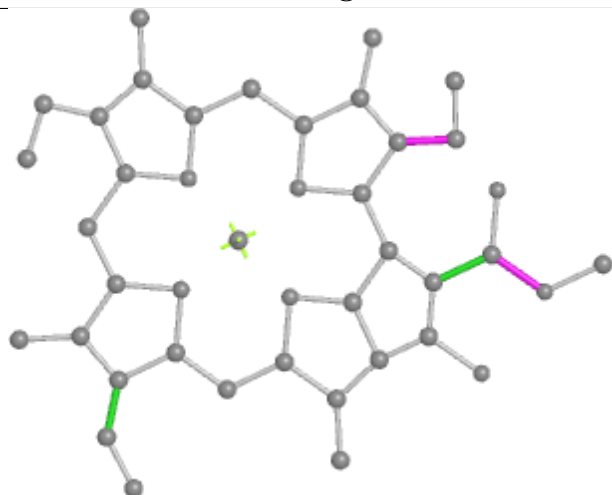
Ligand CLA F2 302



Bond lengths



Bond angles

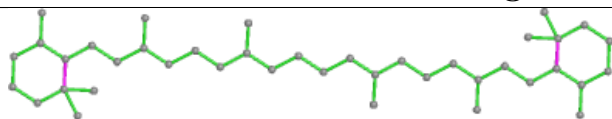


Torsions

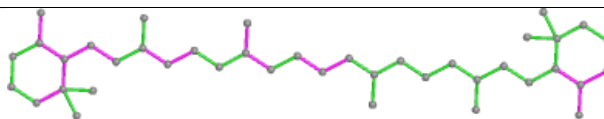


Rings

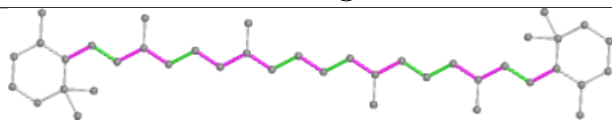
Ligand BCR F2 303



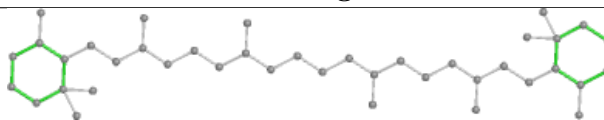
Bond lengths



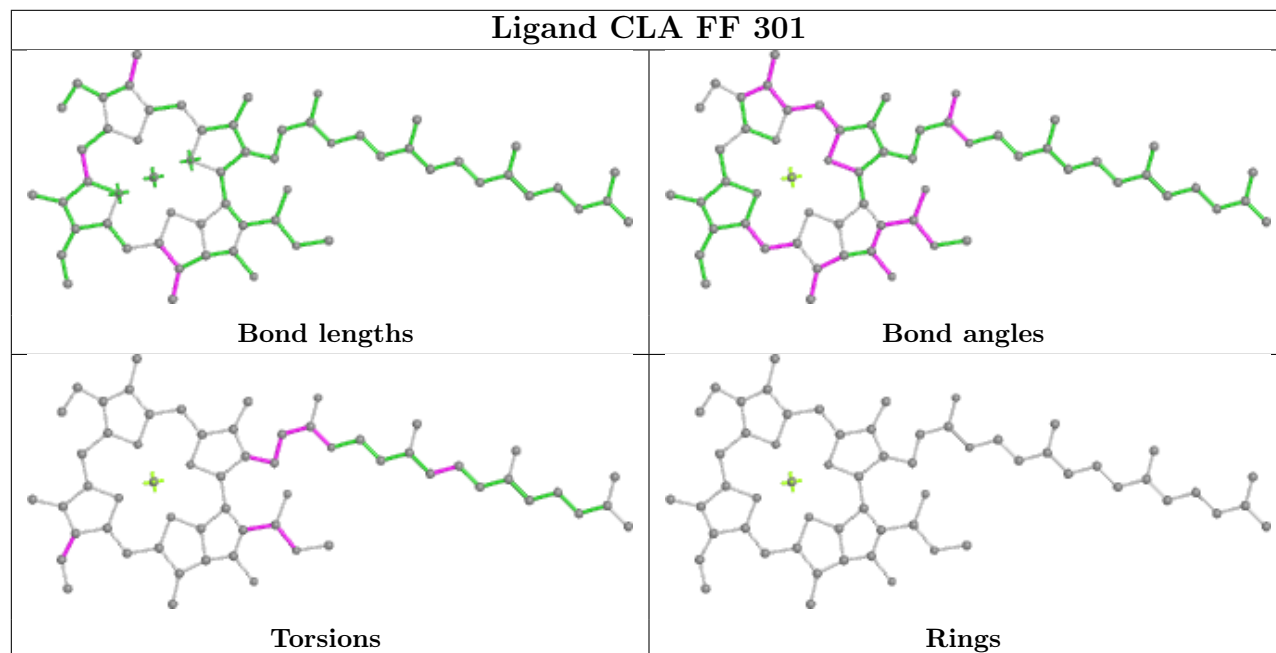
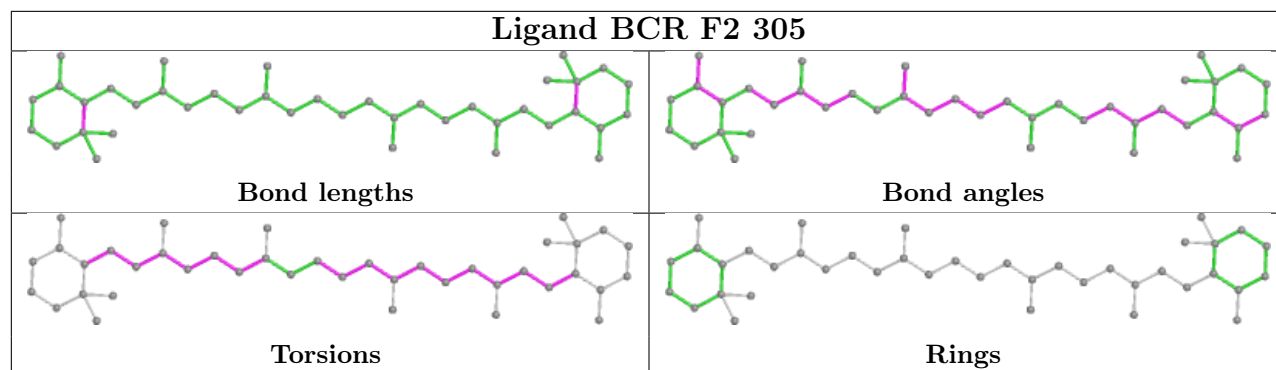
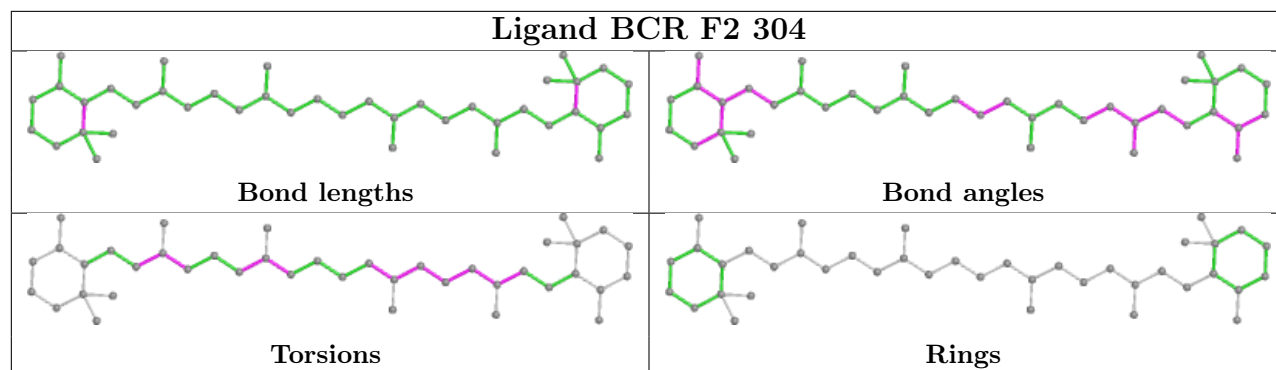
Bond angles



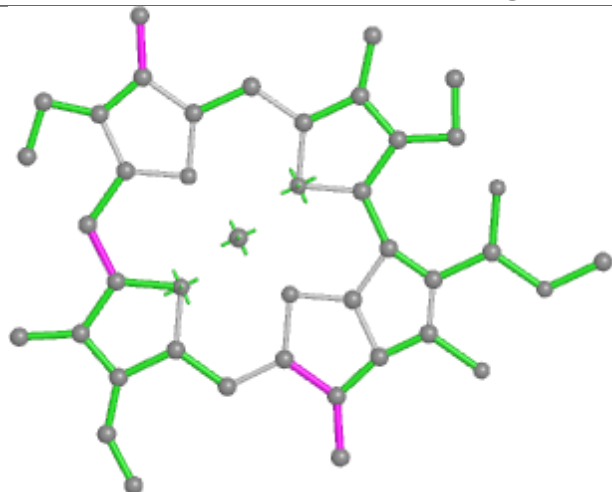
Torsions



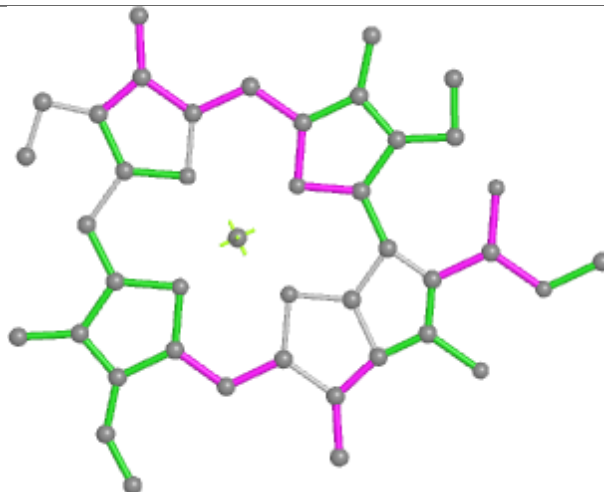
Rings



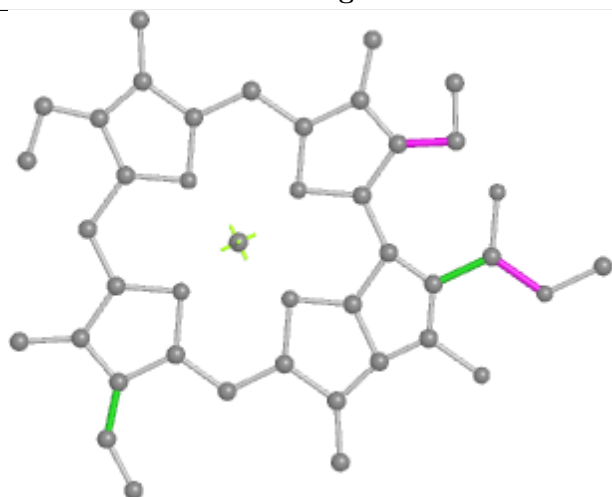
Ligand CLA FF 302



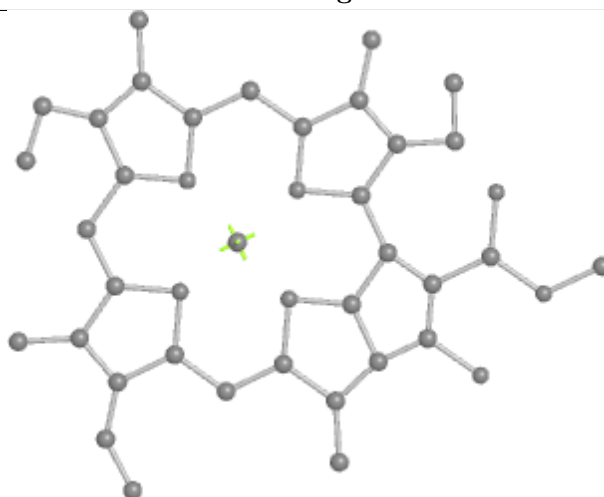
Bond lengths



Bond angles

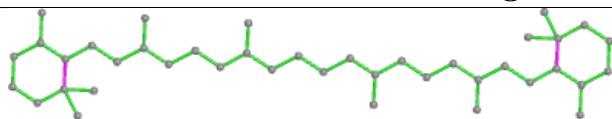


Torsions

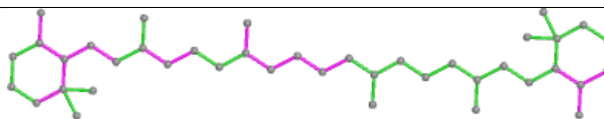


Rings

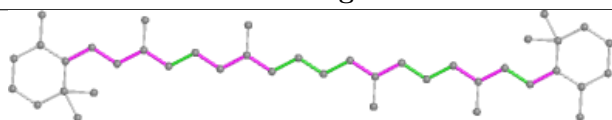
Ligand BCR FF 303



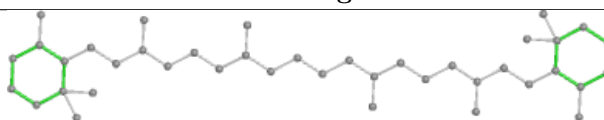
Bond lengths



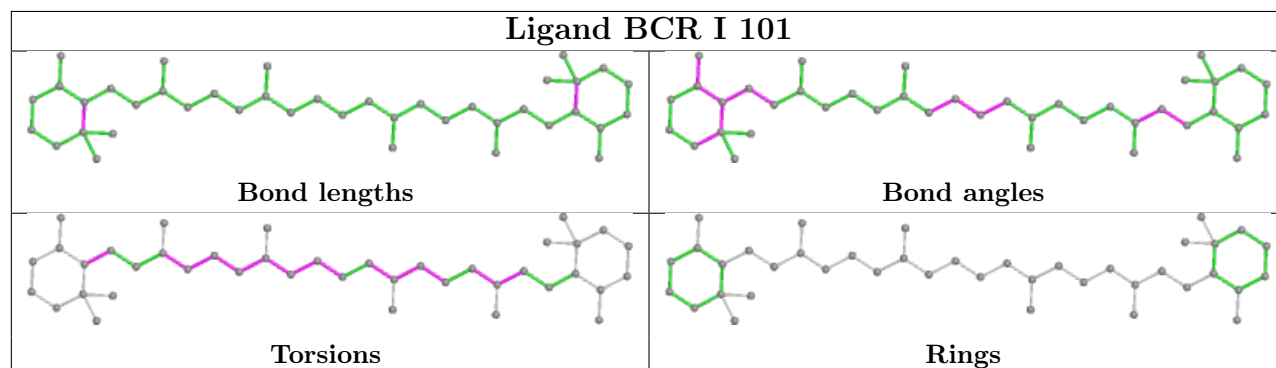
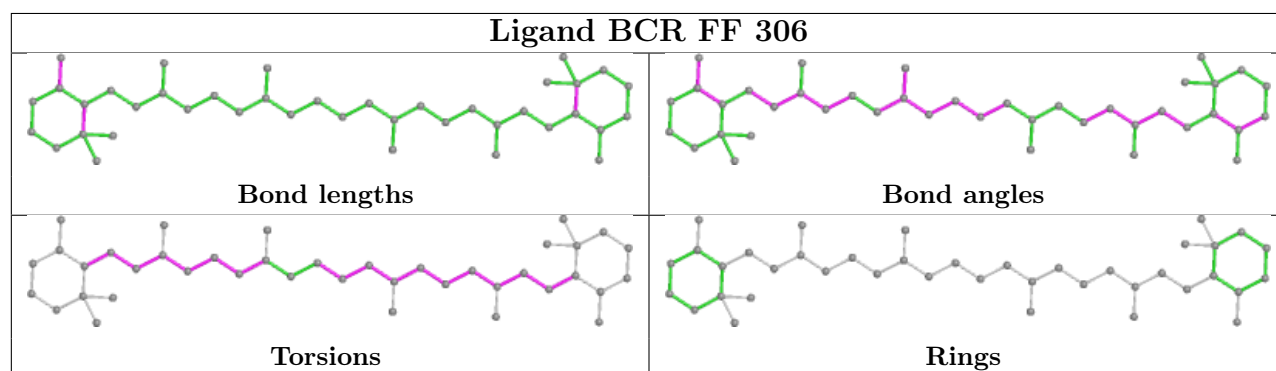
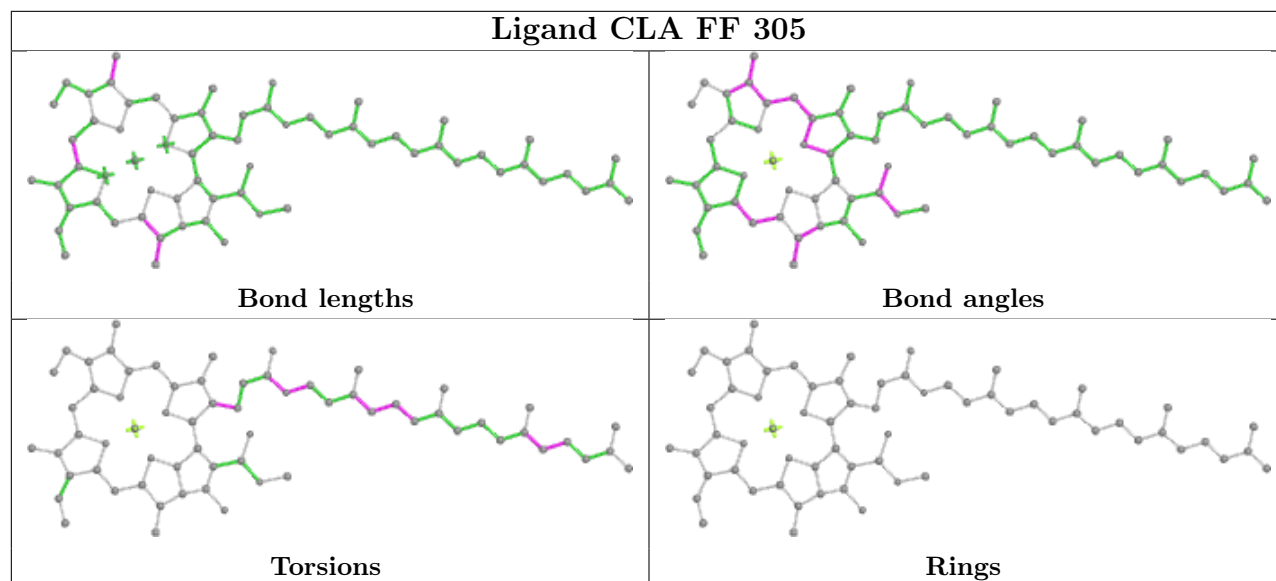
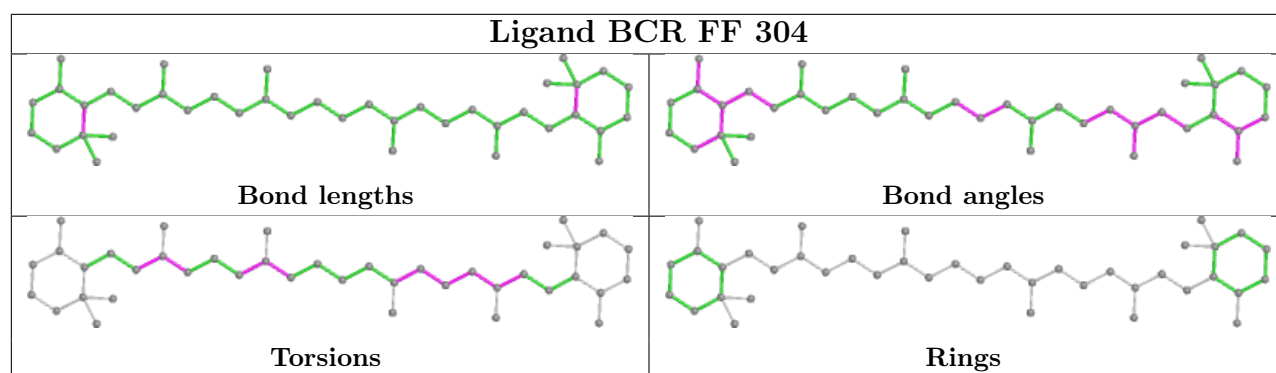
Bond angles

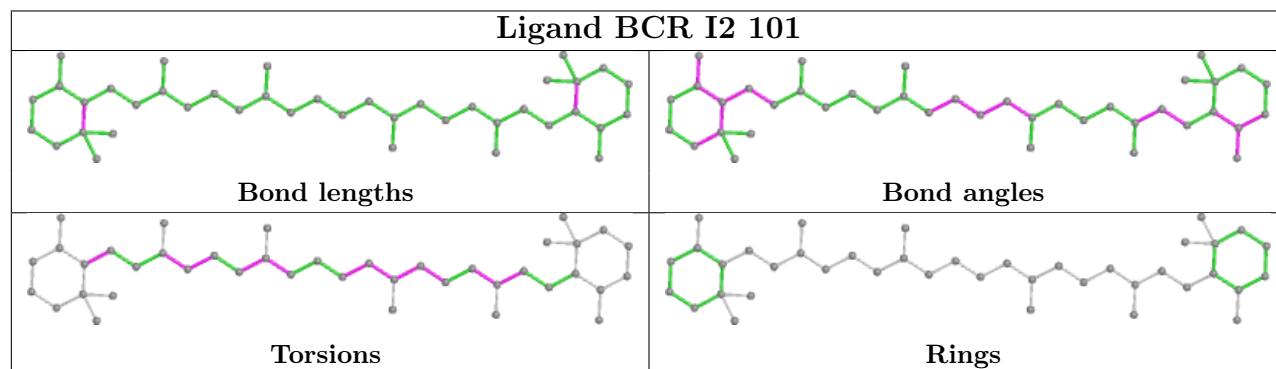
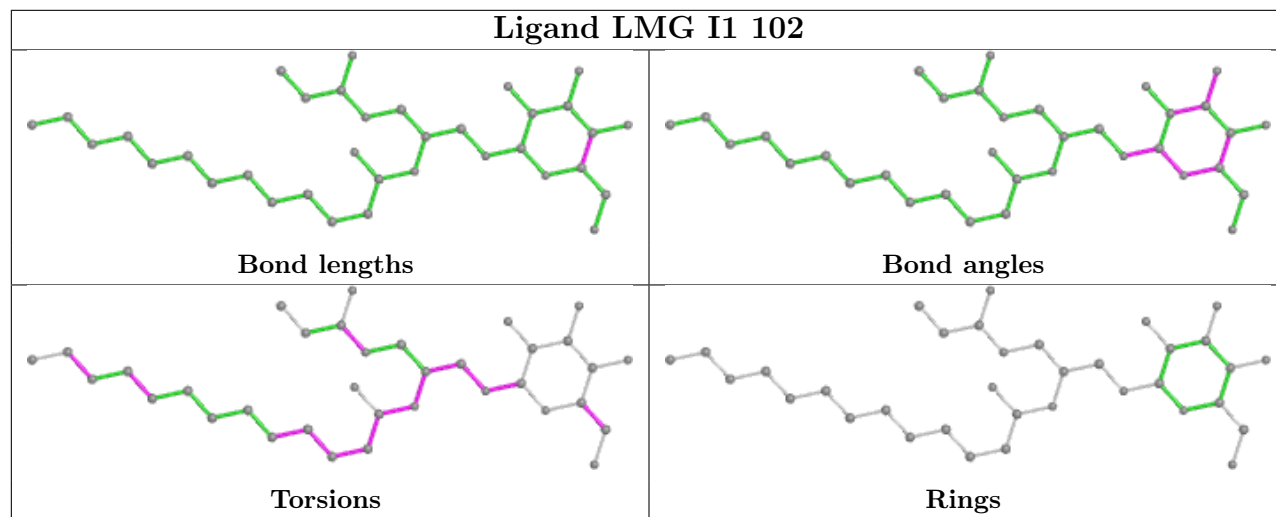
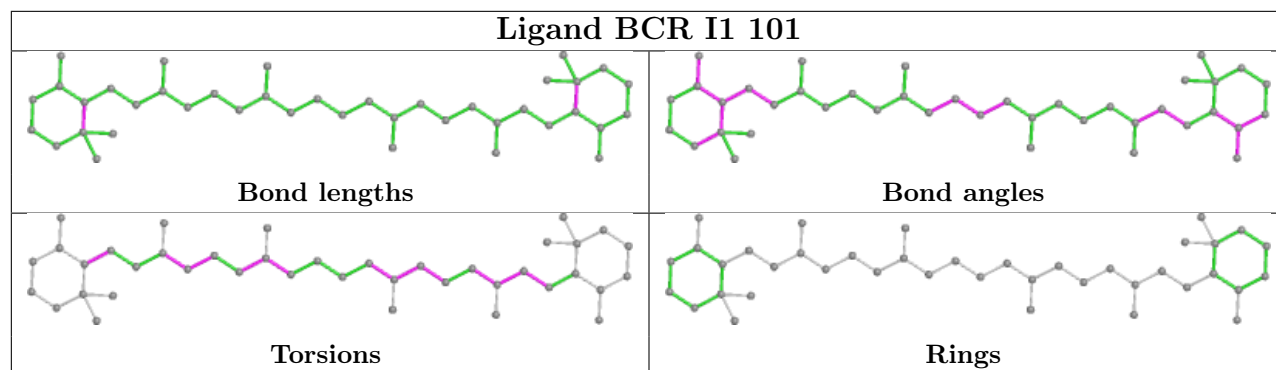
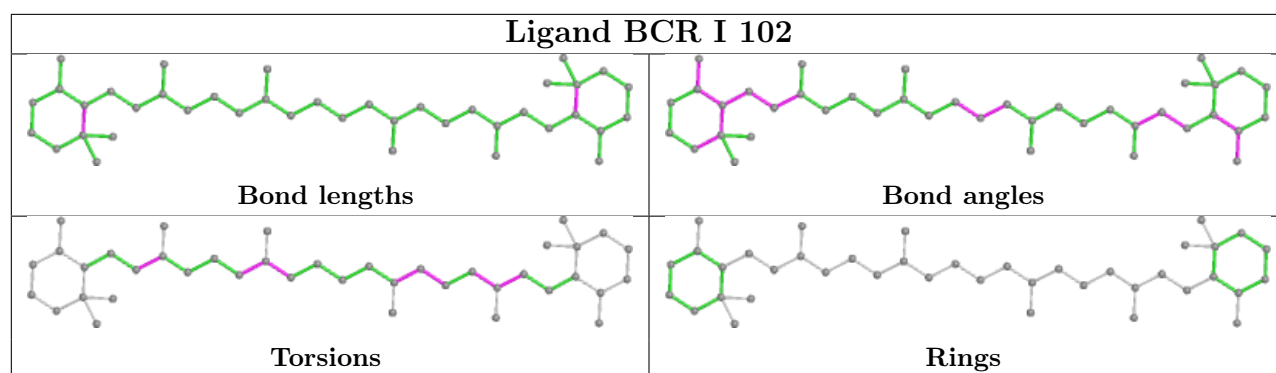


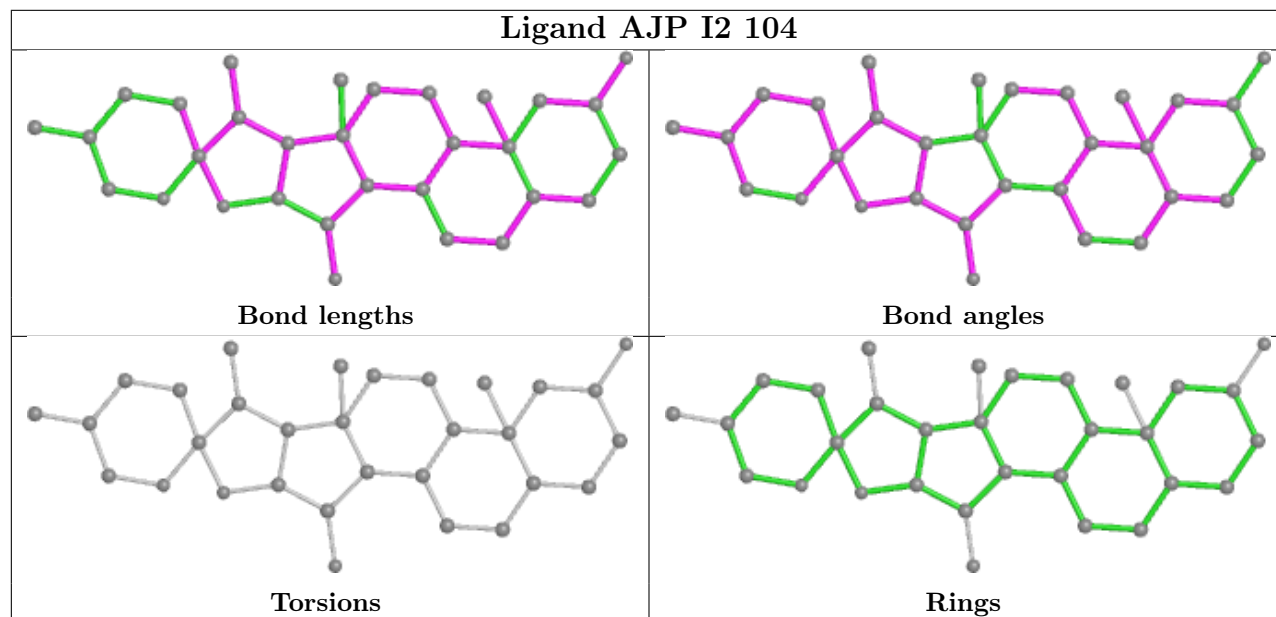
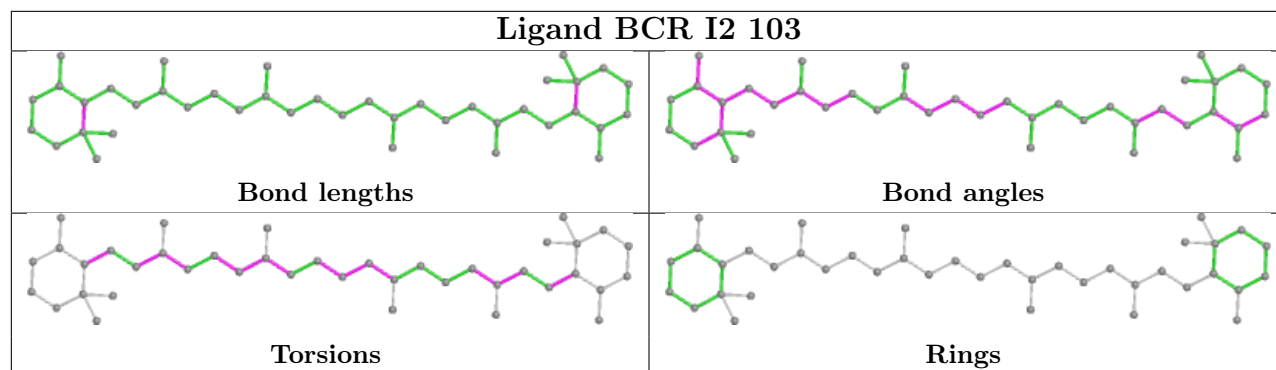
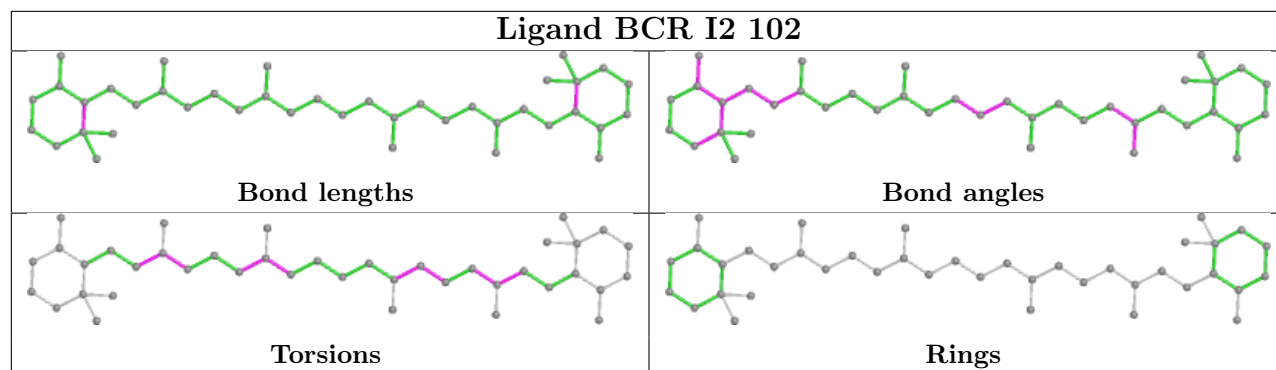
Torsions

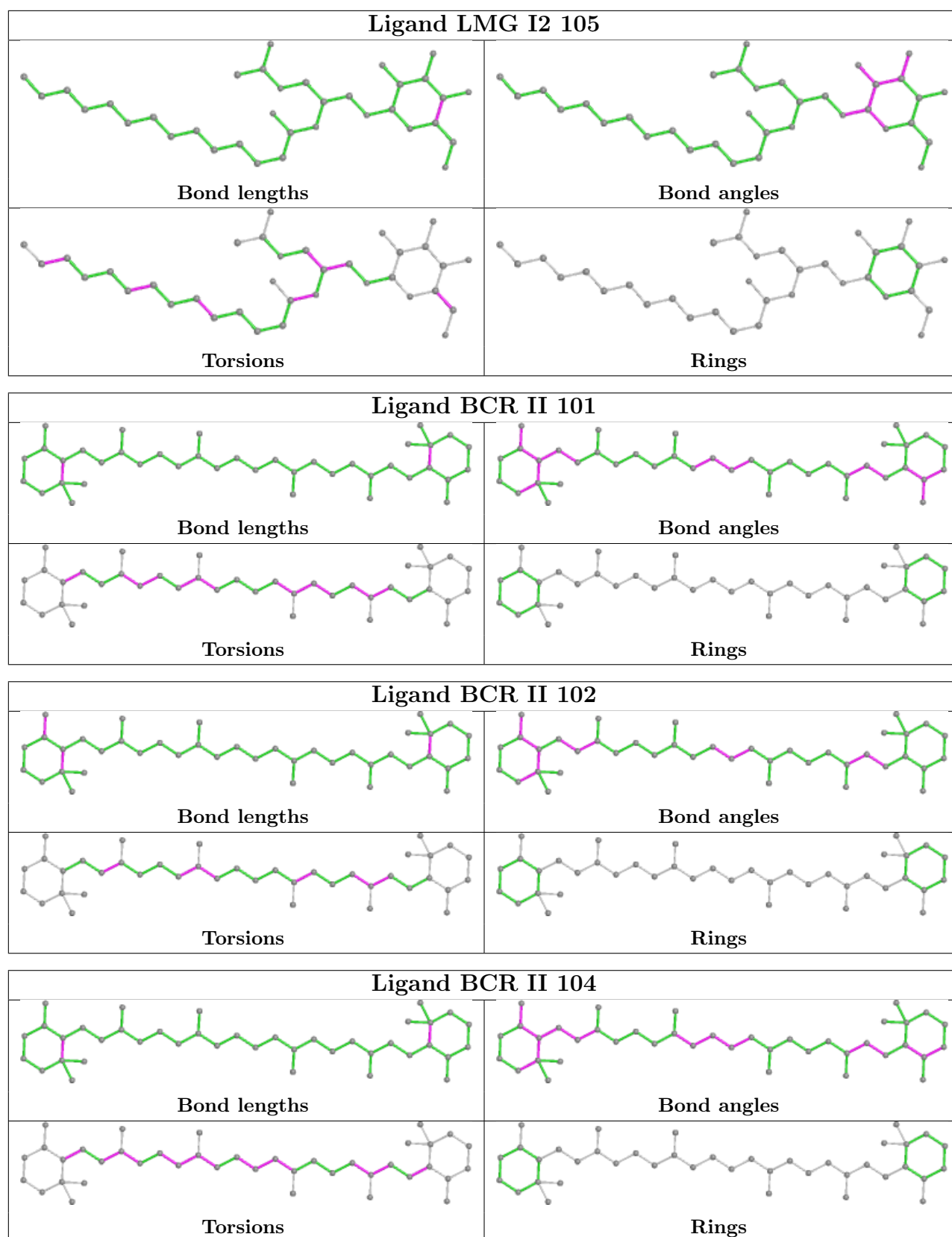


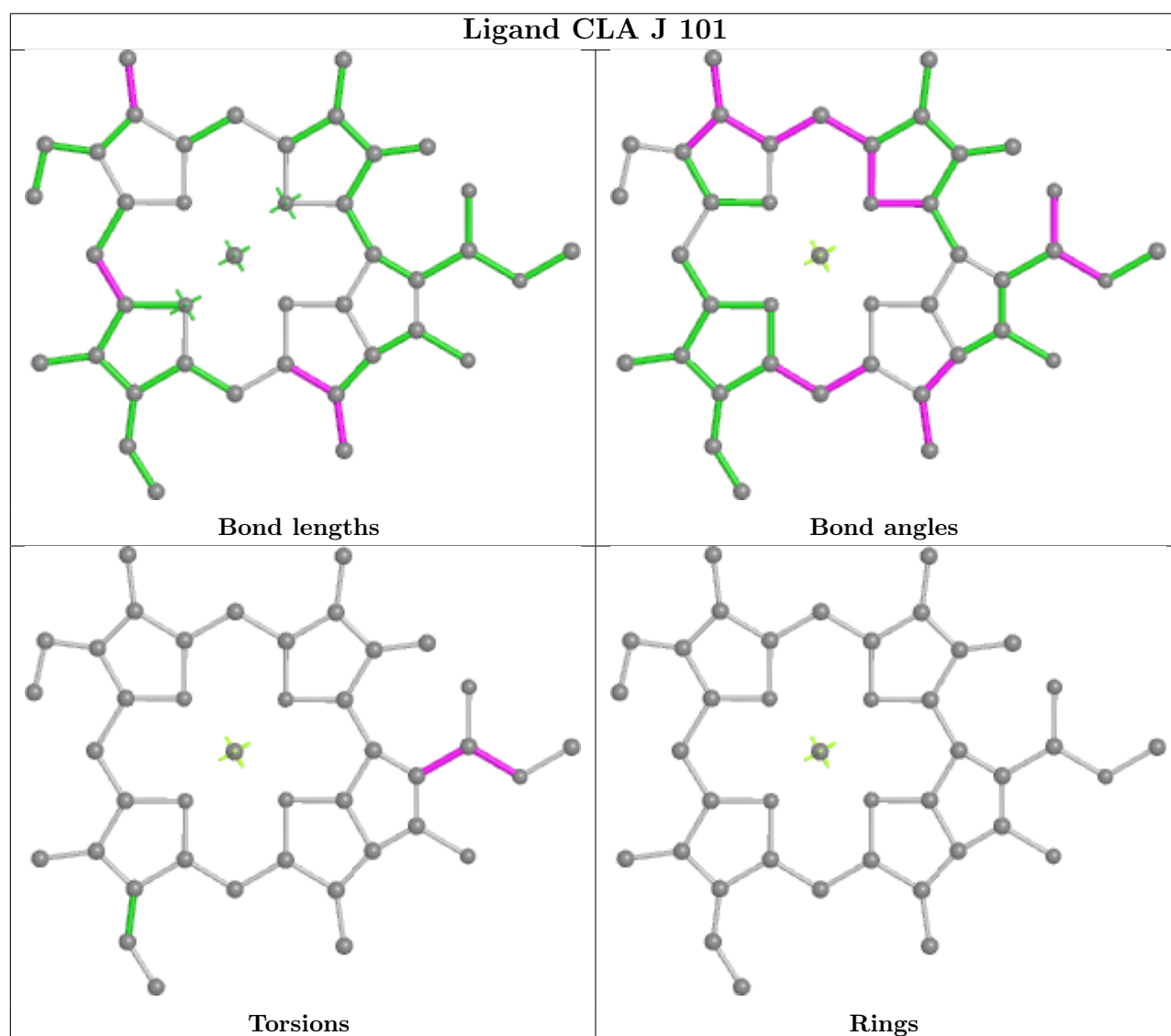
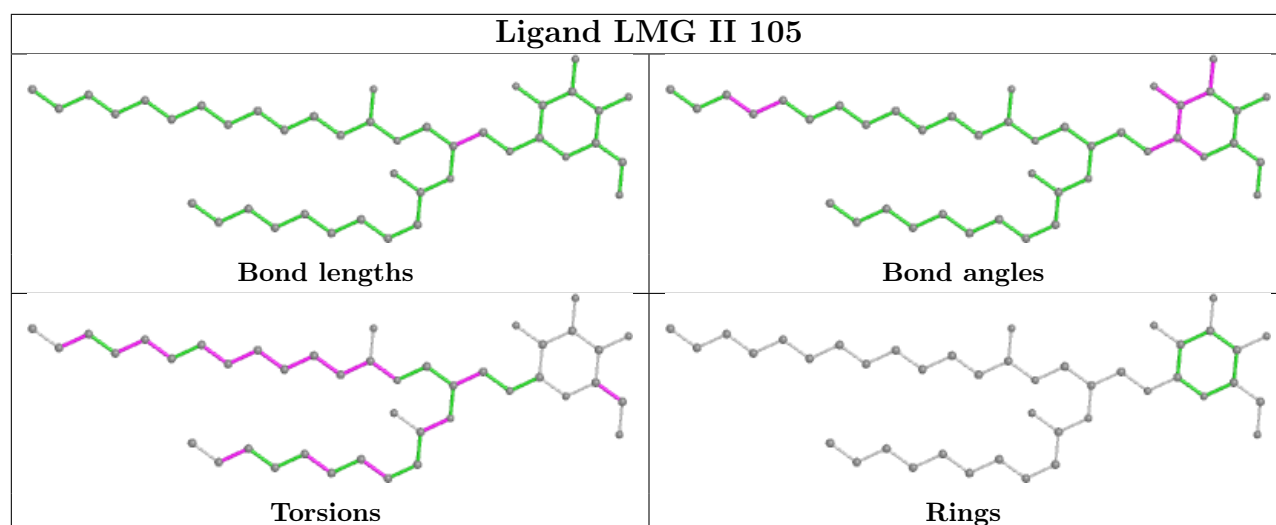
Rings

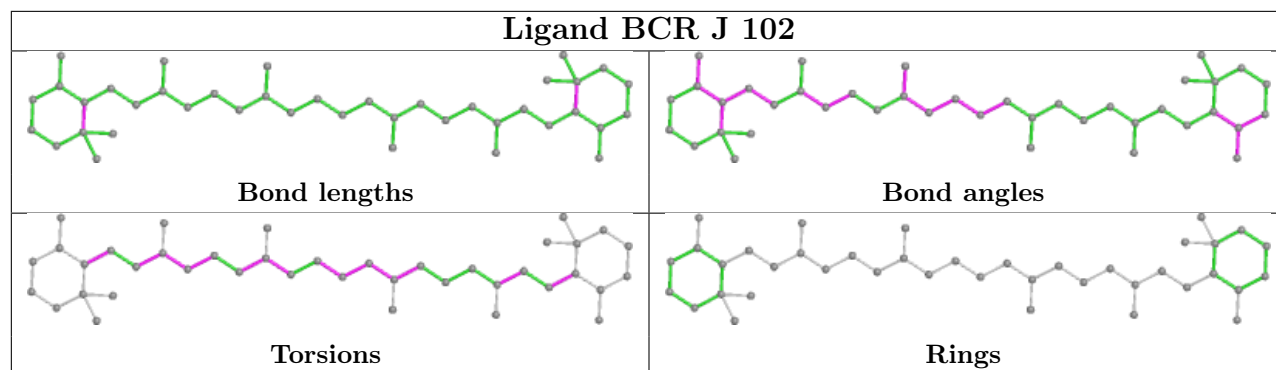
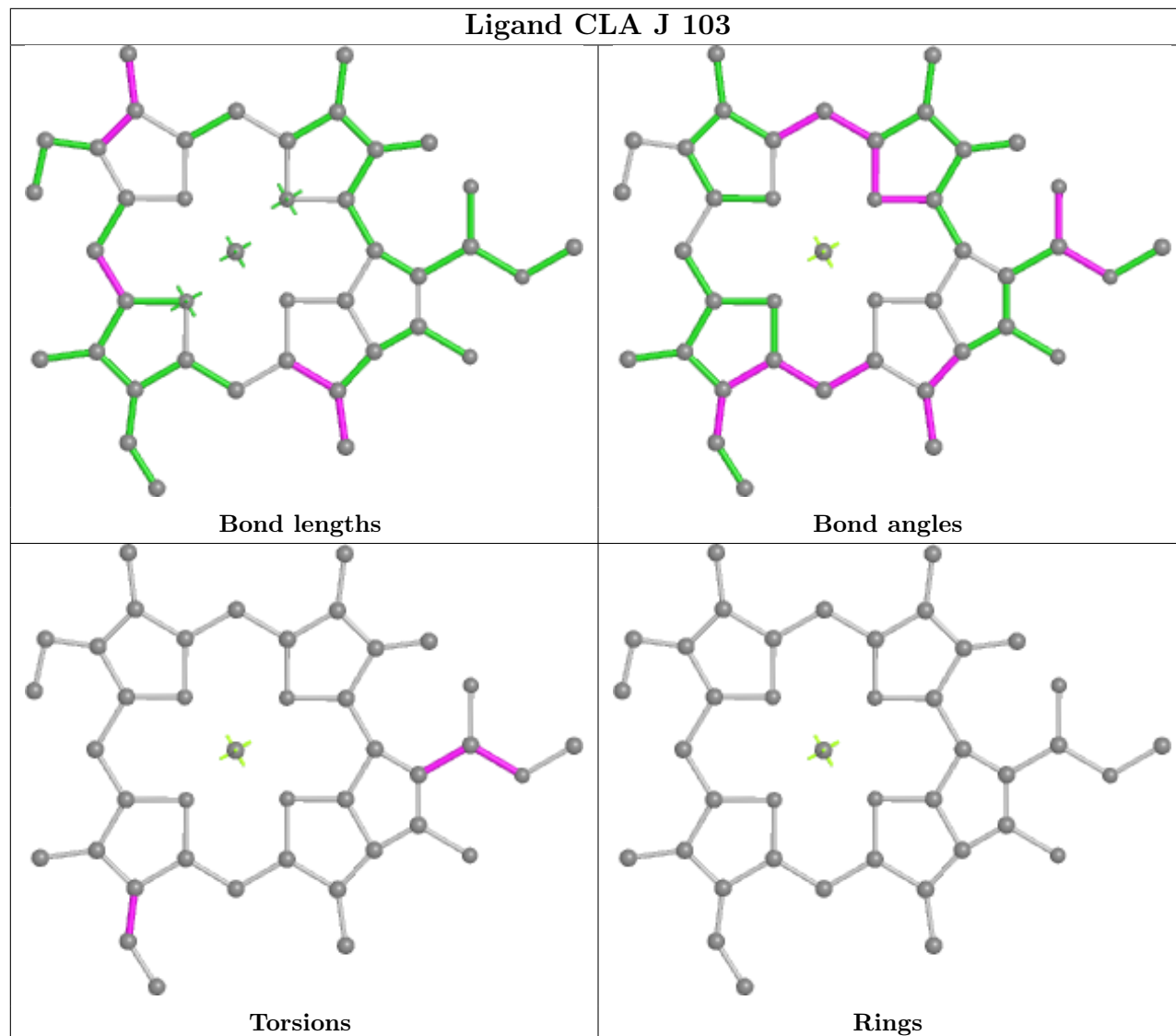


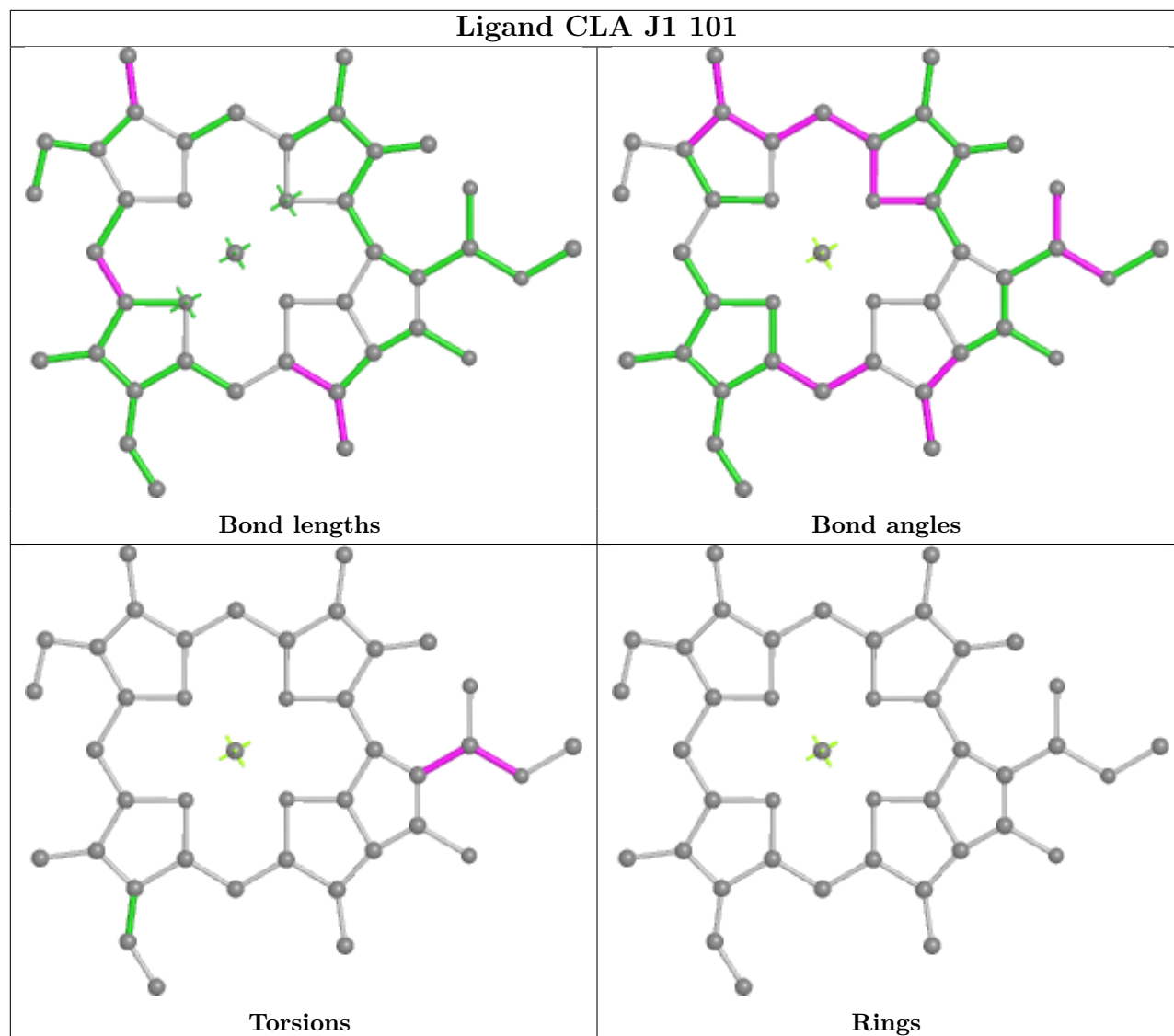
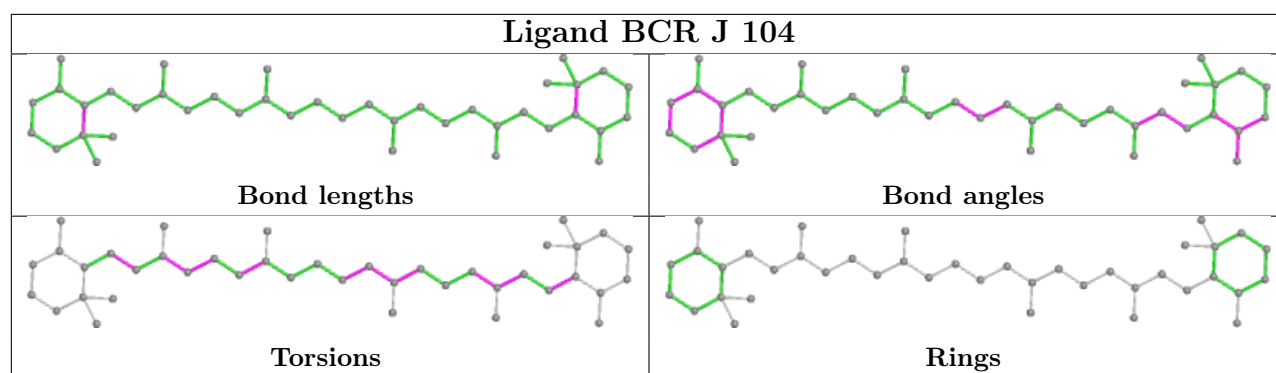


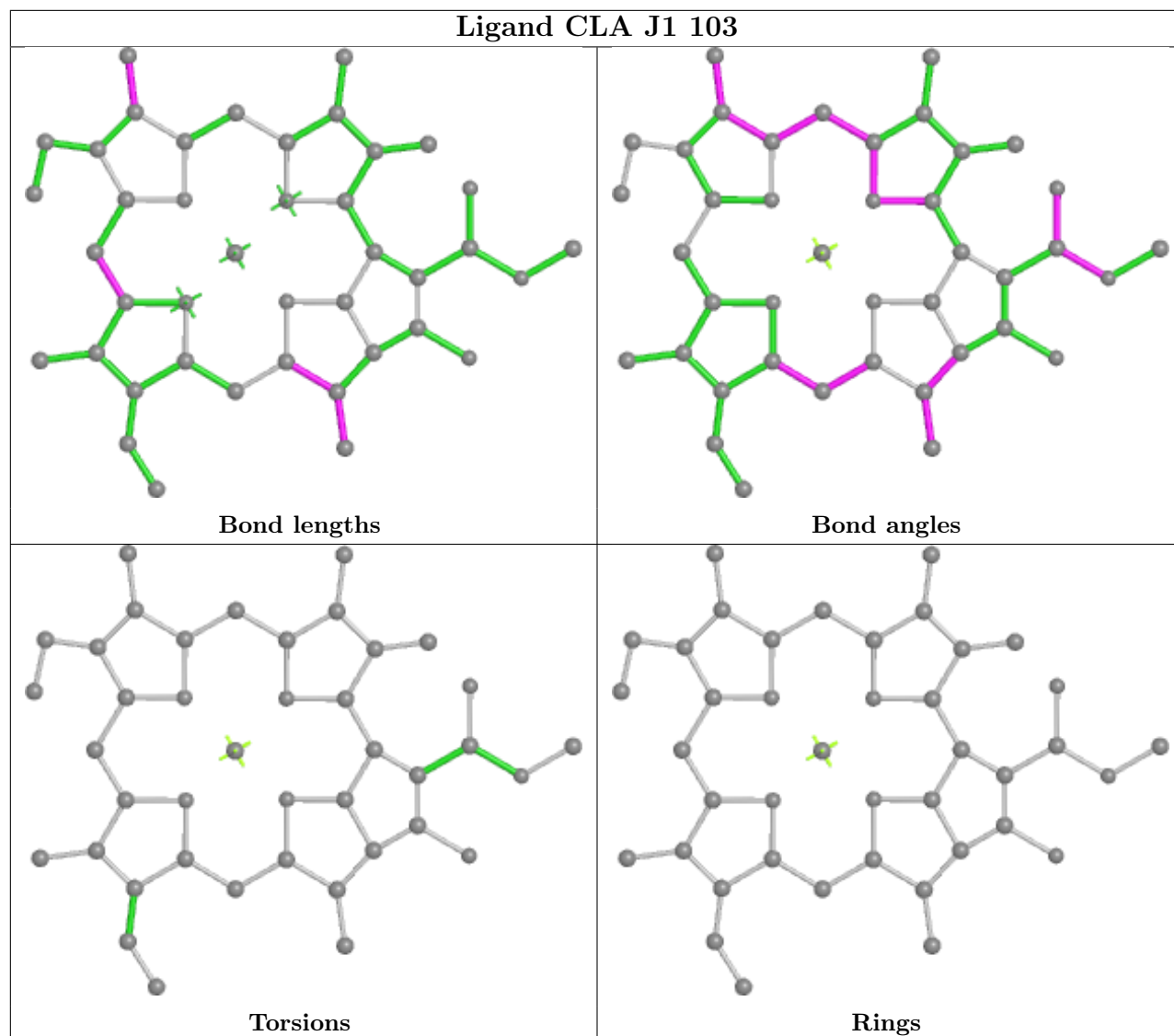
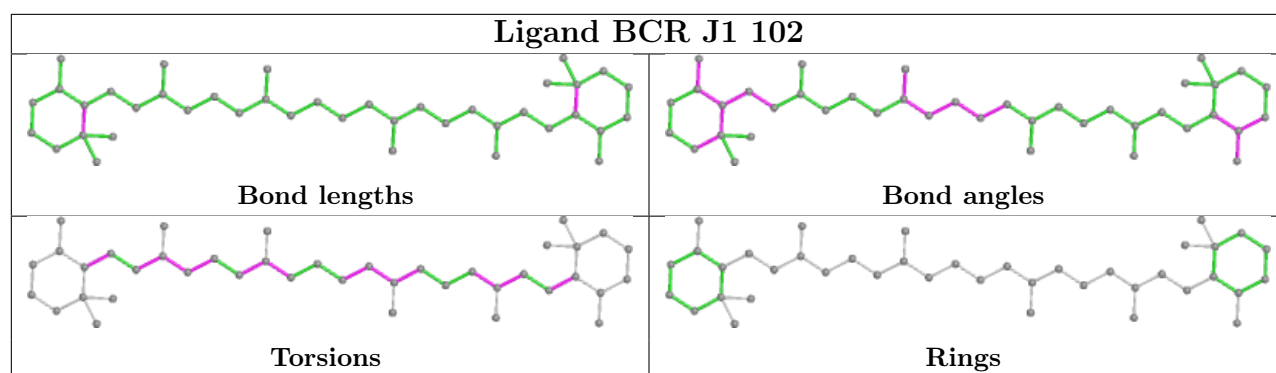


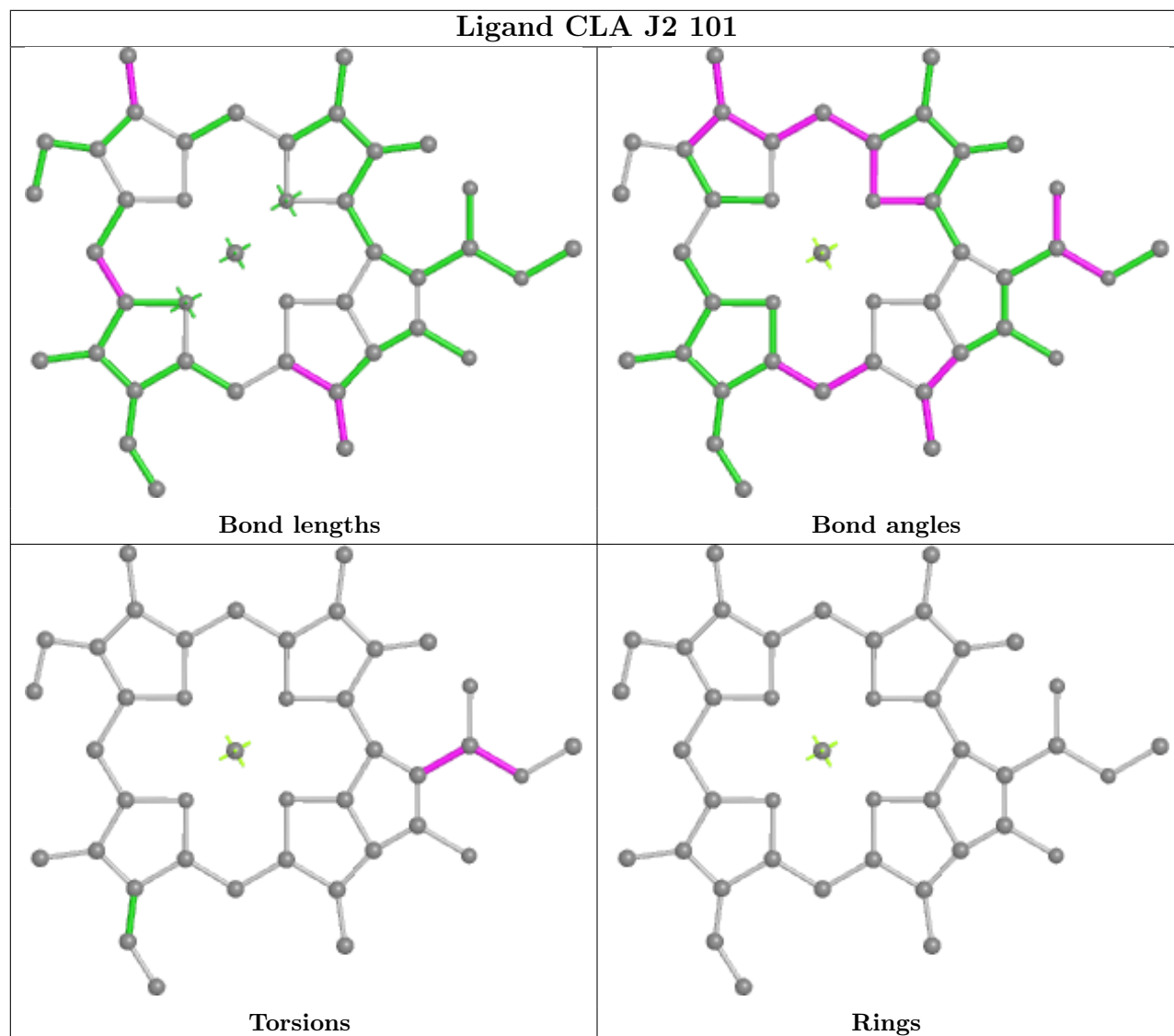
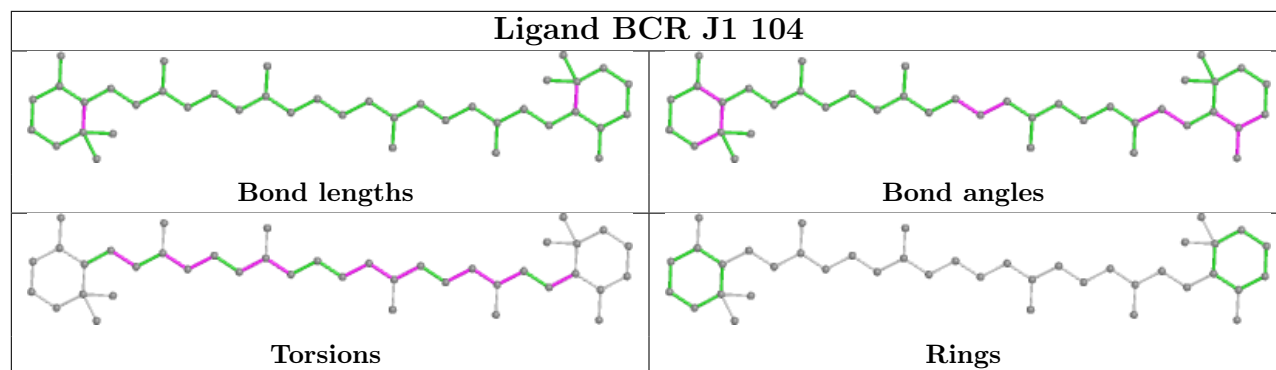


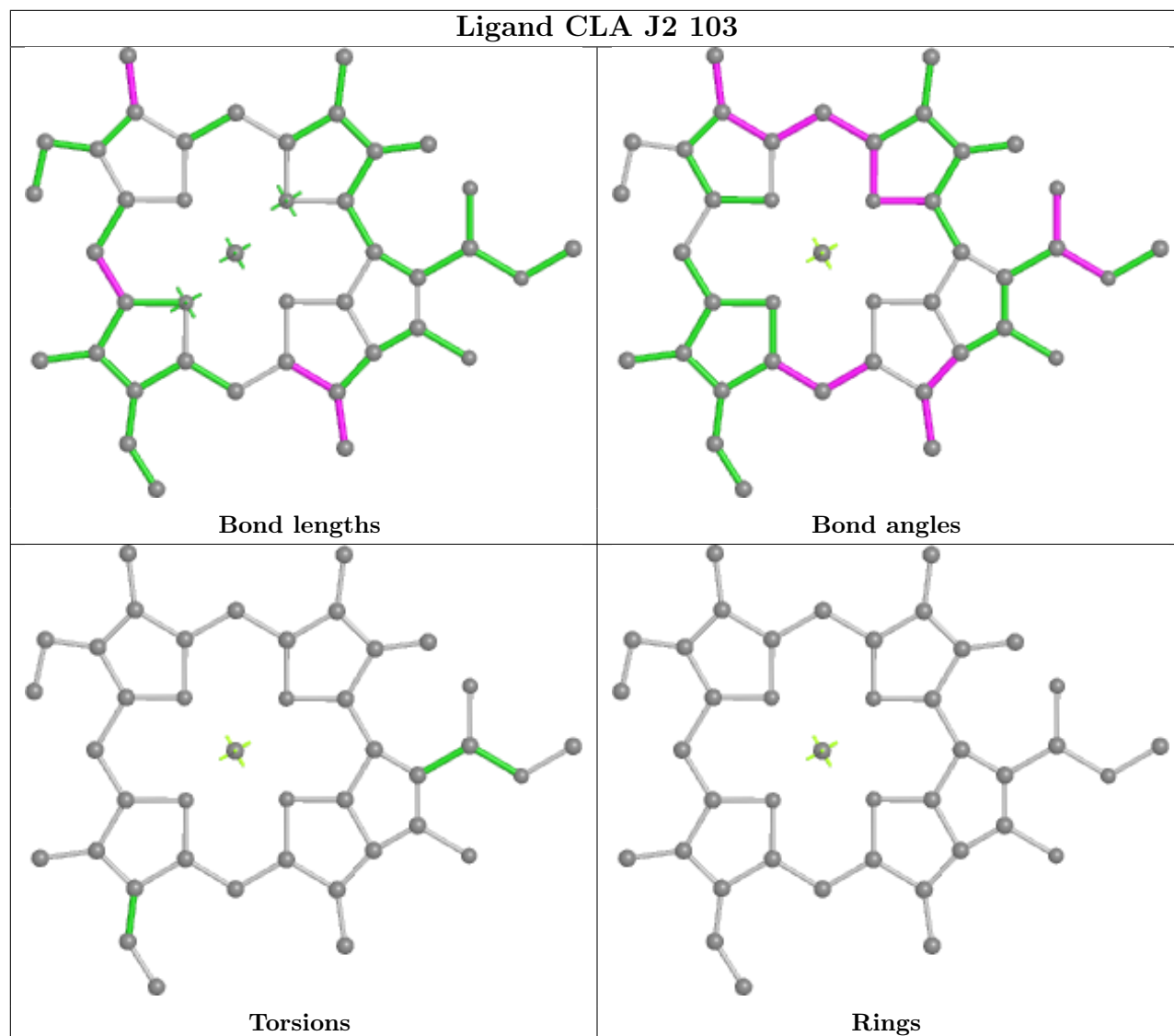
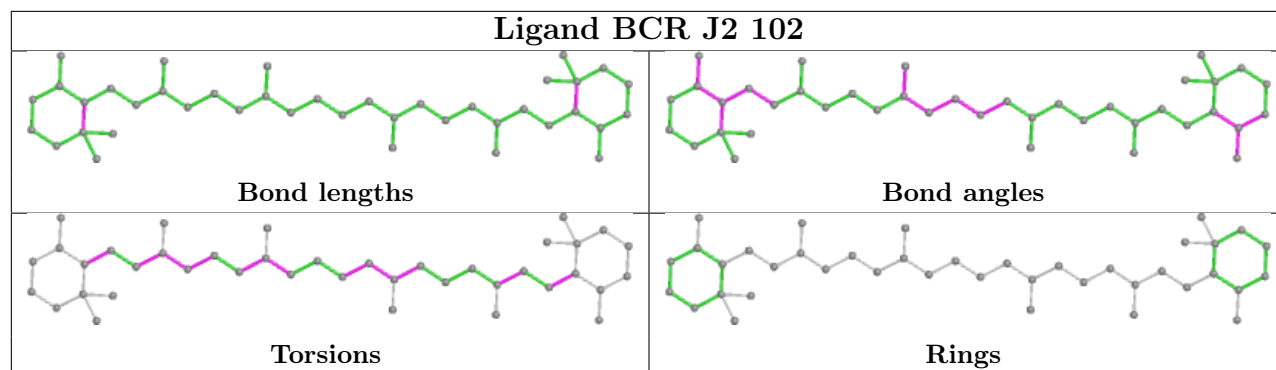


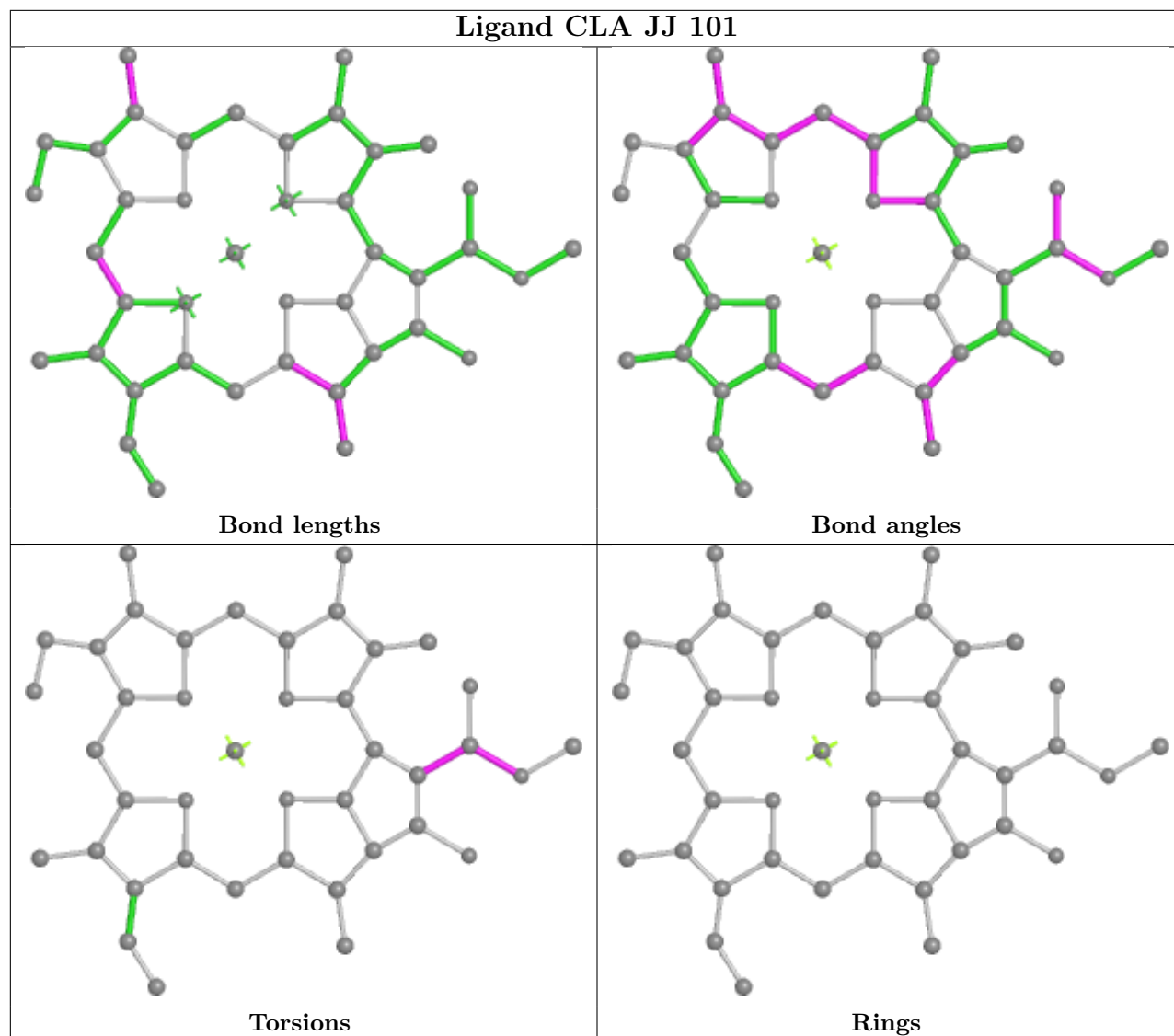
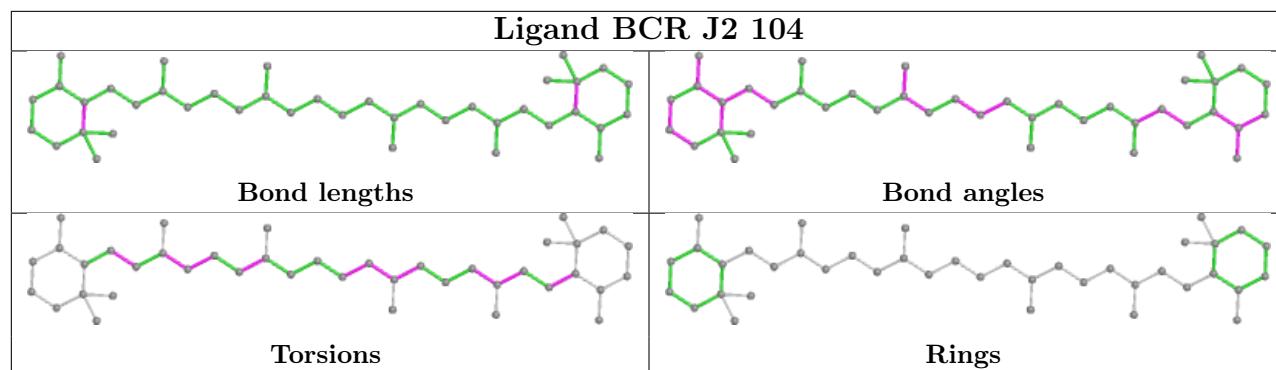
Ligand BCR J 102**Ligand CLA J 103**

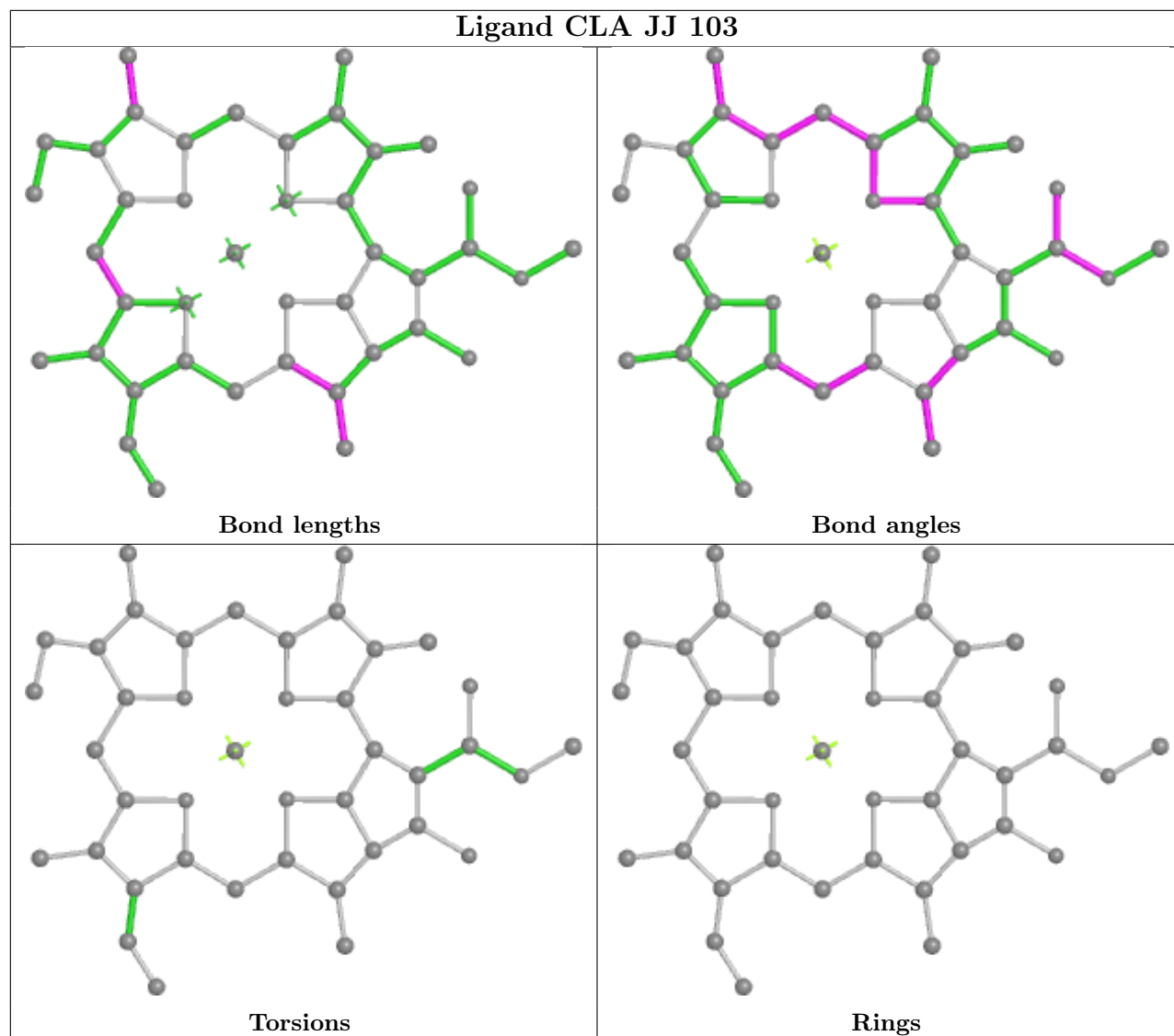
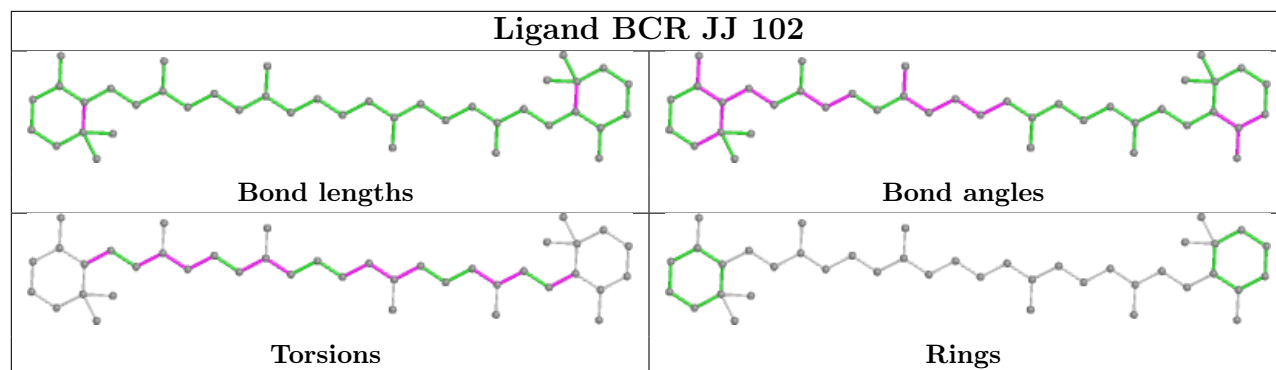


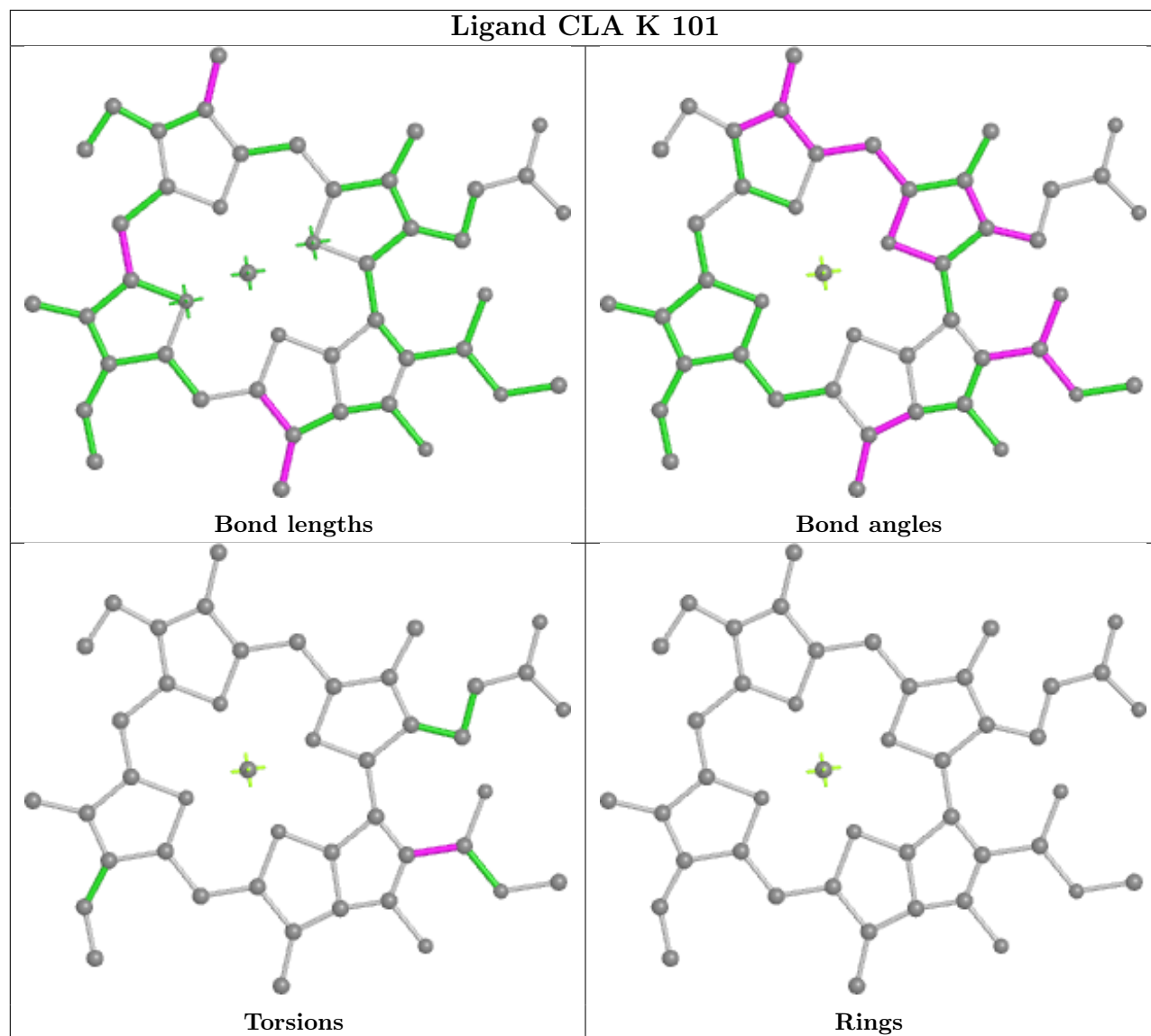
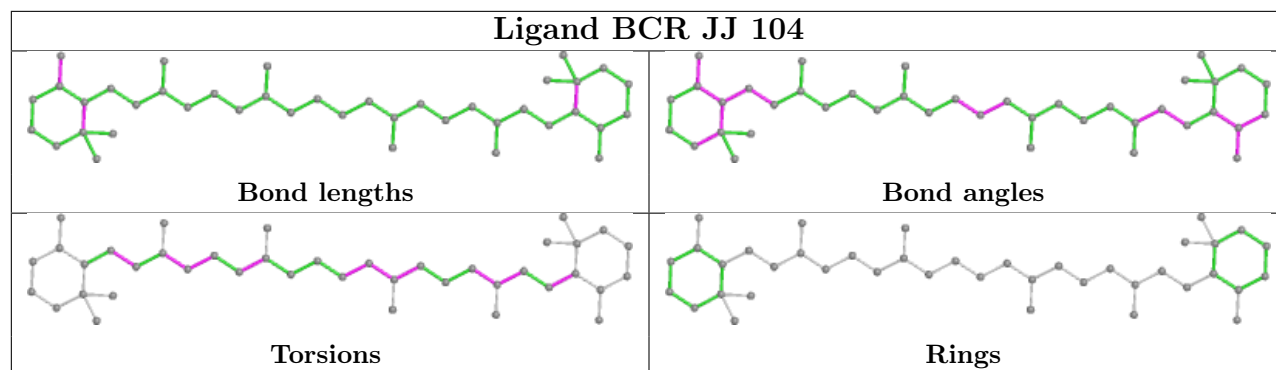




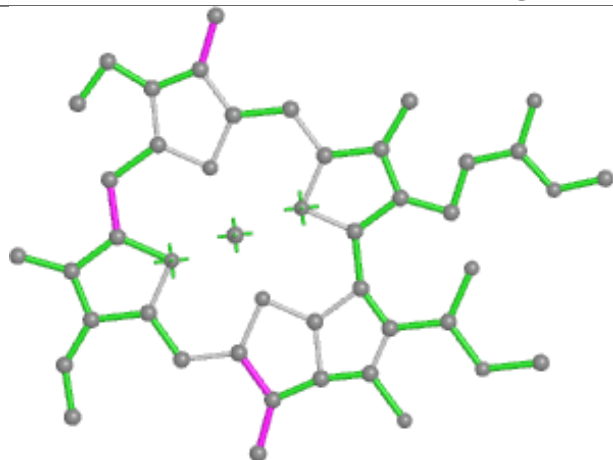




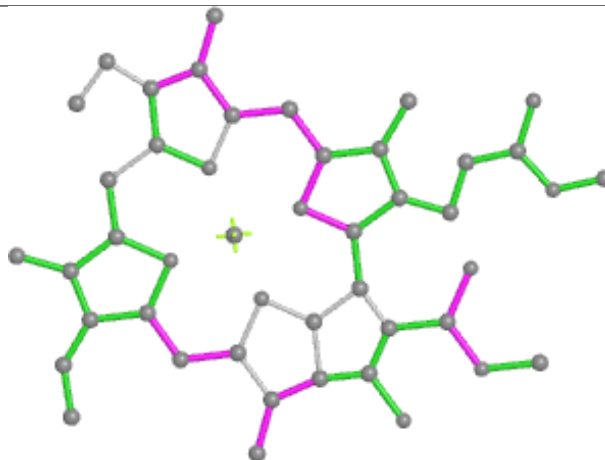




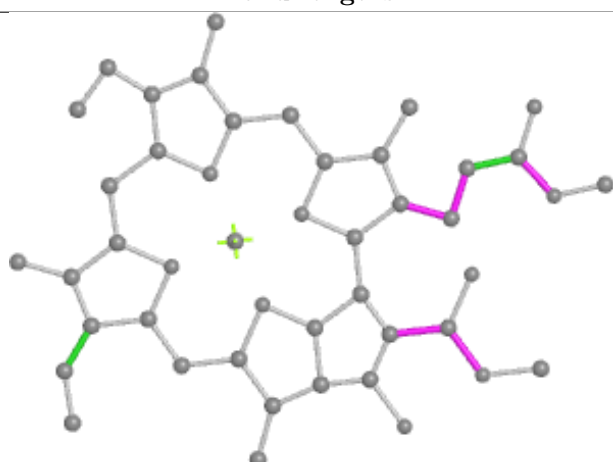
Ligand CLA K 102



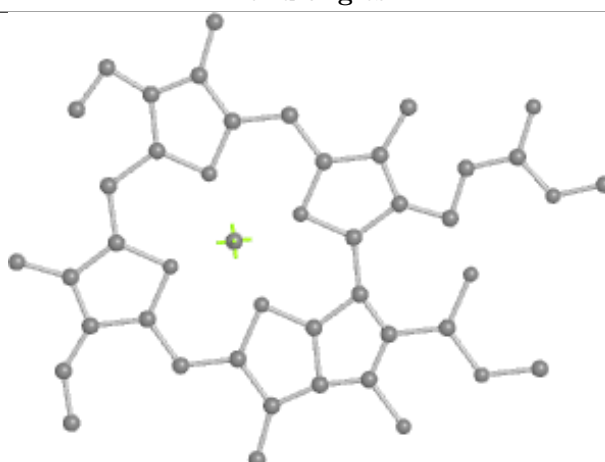
Bond lengths



Bond angles

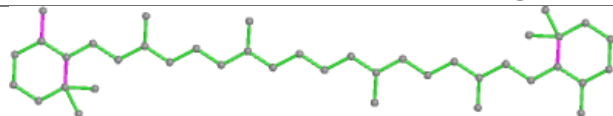


Torsions

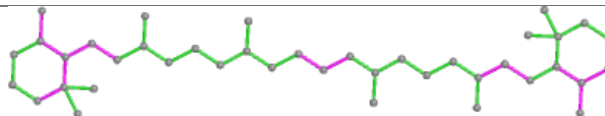


Rings

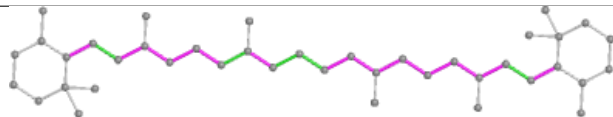
Ligand BCR K 103



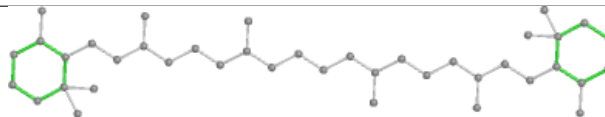
Bond lengths



Bond angles

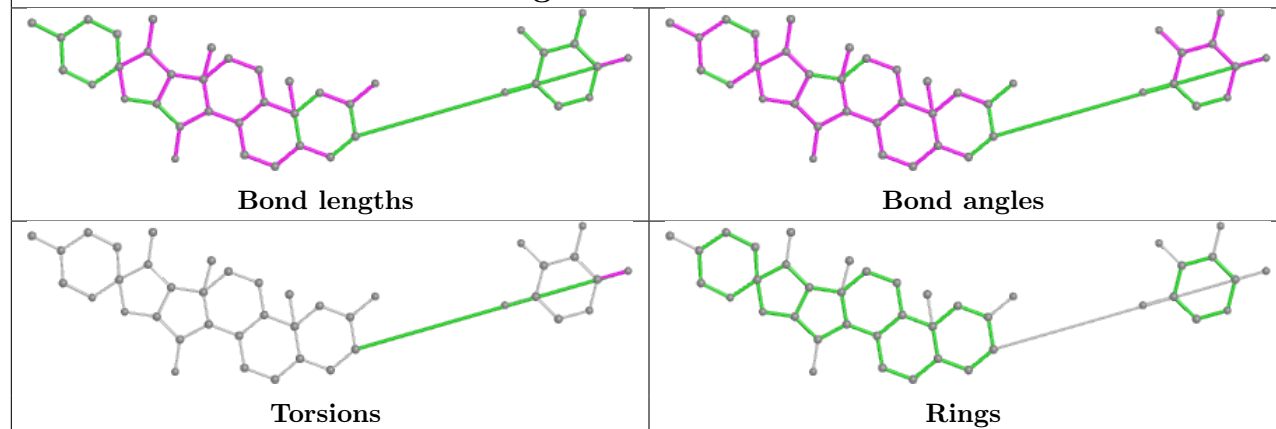


Torsions

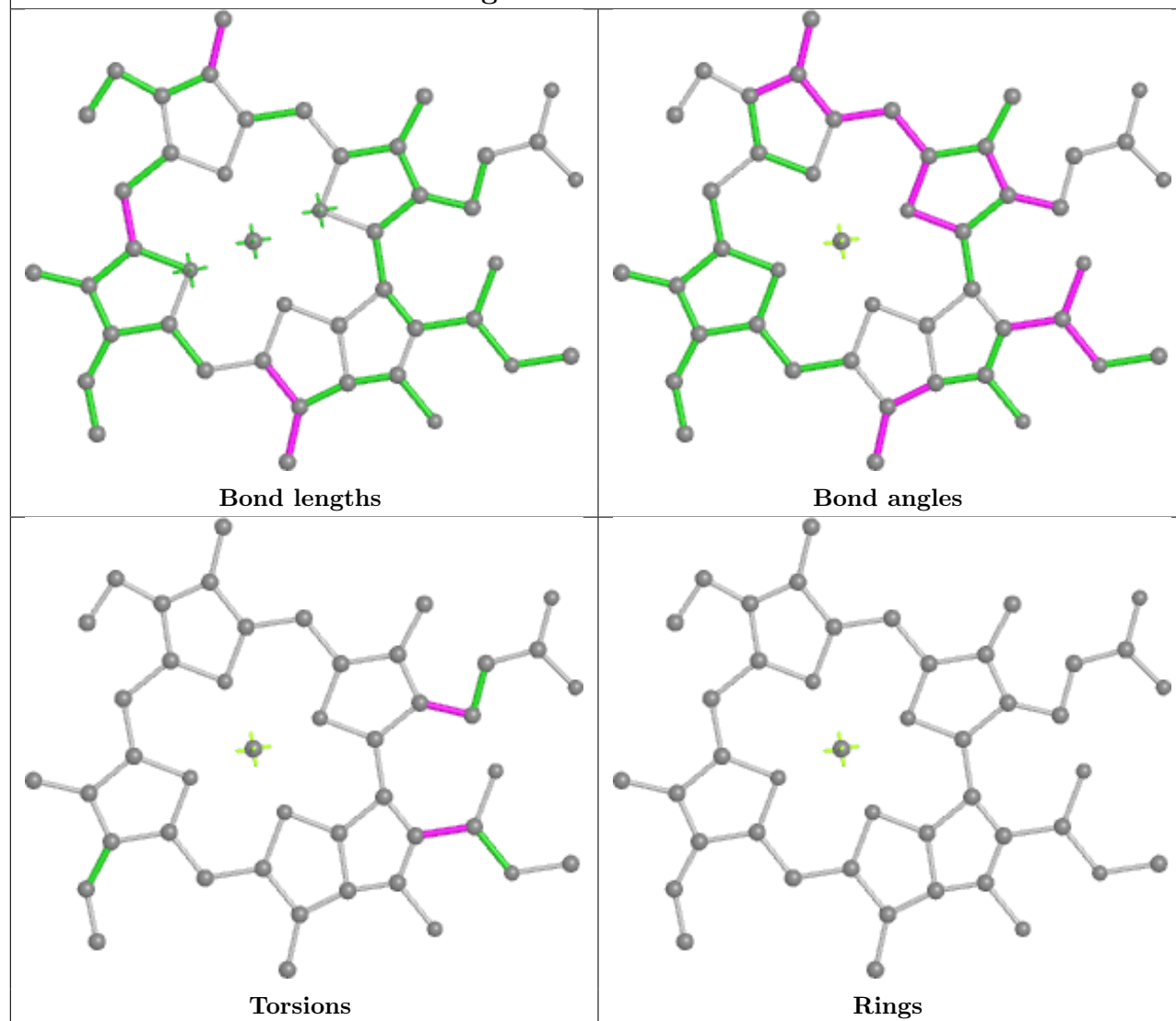


Rings

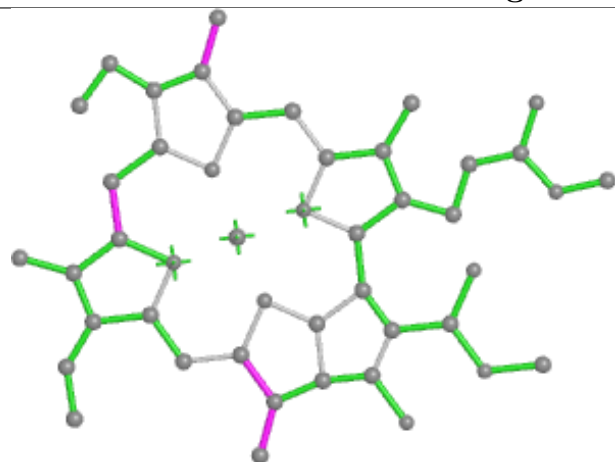
Ligand AJP K 104



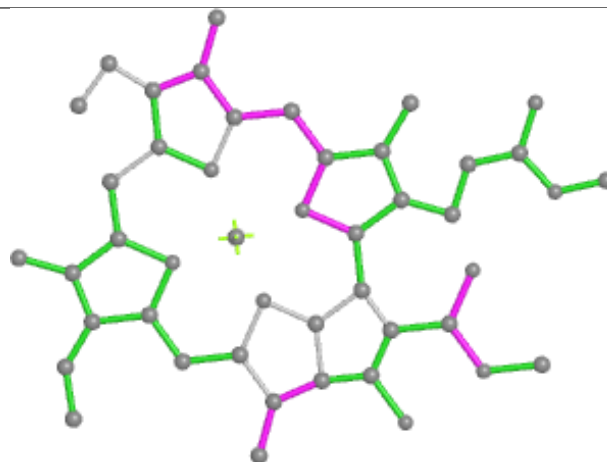
Ligand CLA K1 102



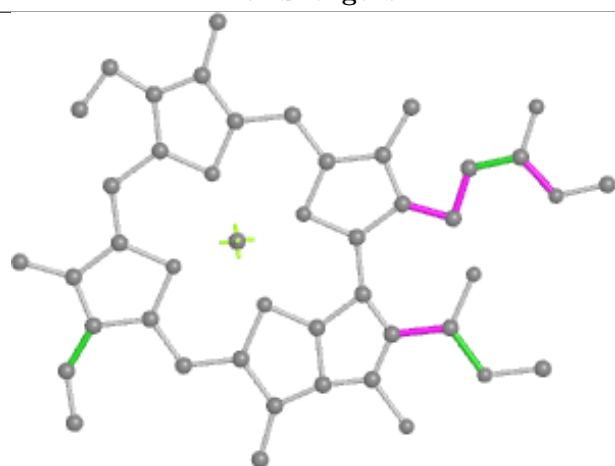
Ligand CLA K1 103



Bond lengths



Bond angles

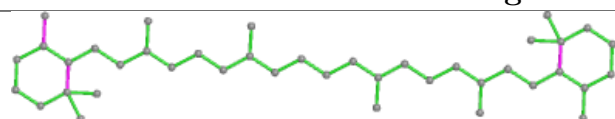


Torsions

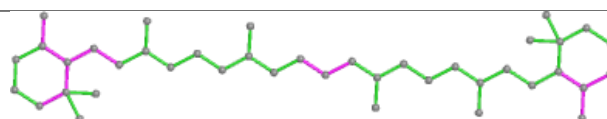


Rings

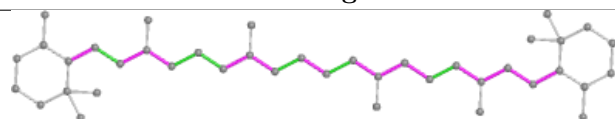
Ligand BCR K1 104



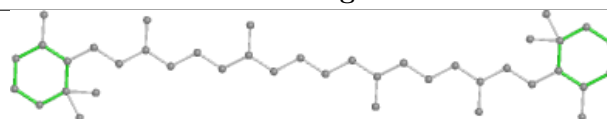
Bond lengths



Bond angles

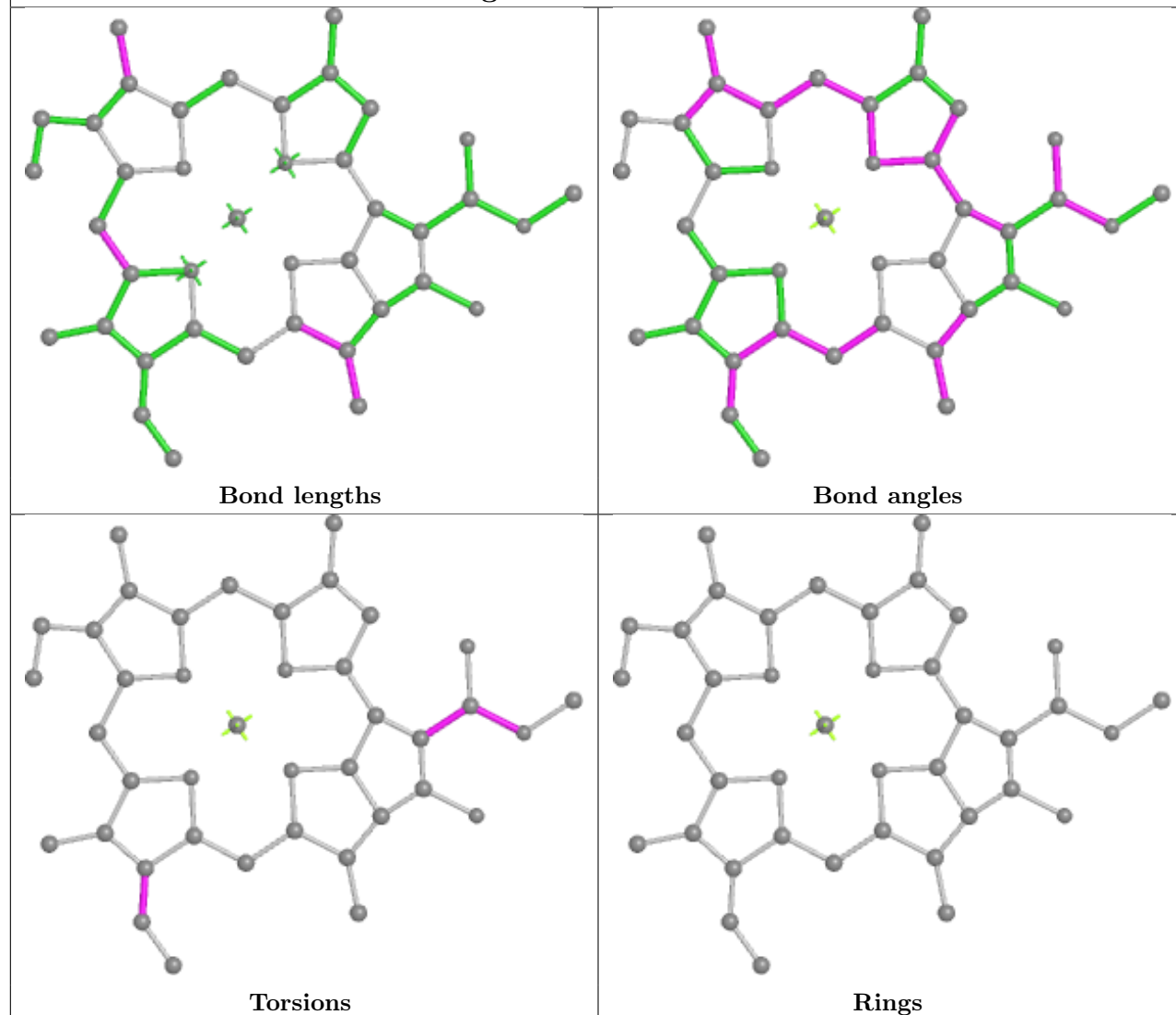


Torsions

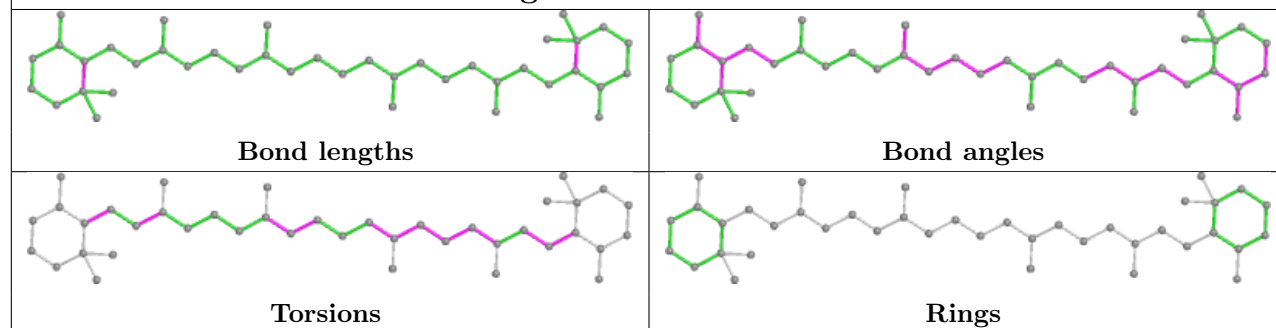


Rings

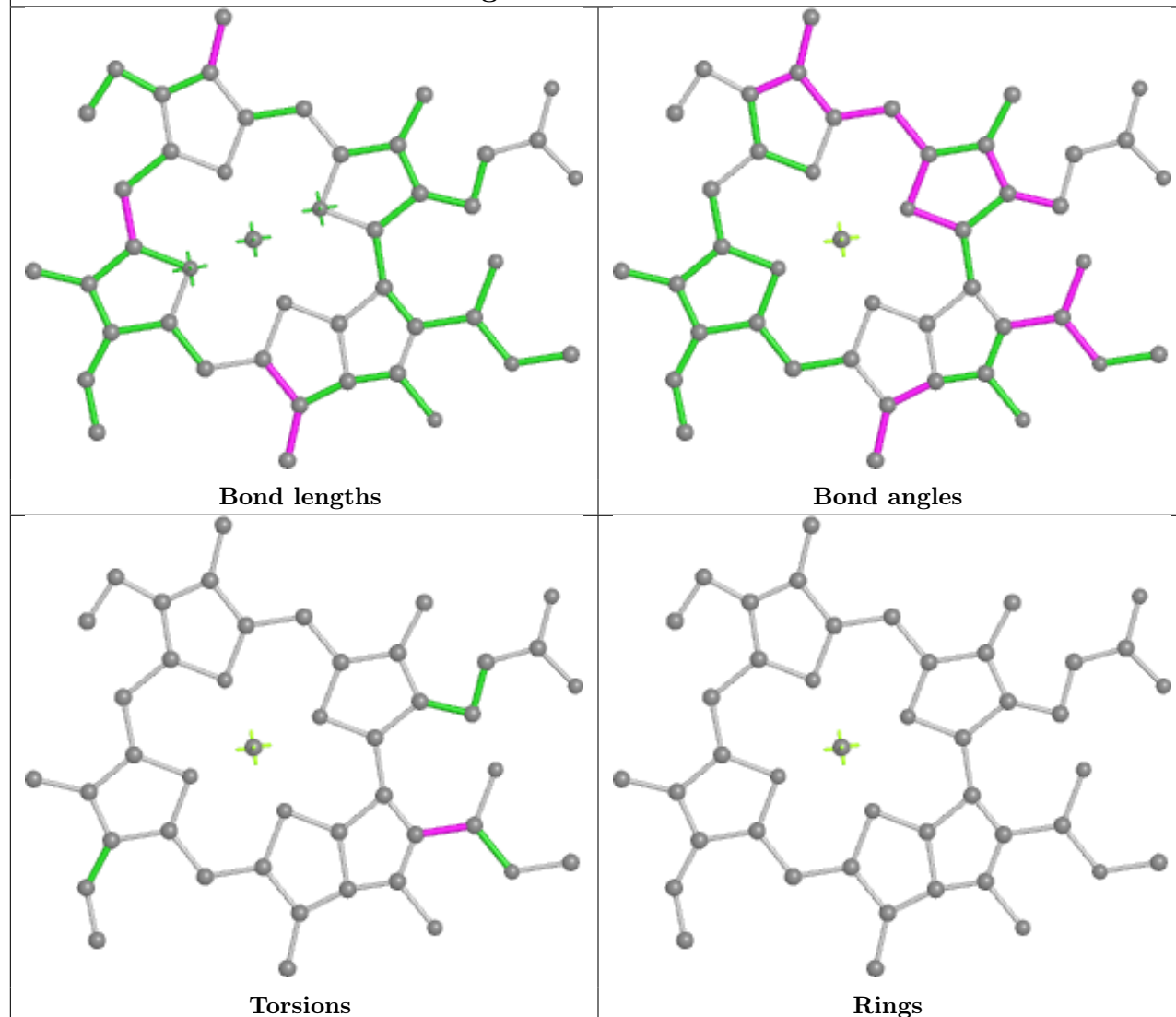
Ligand CLA K1 105



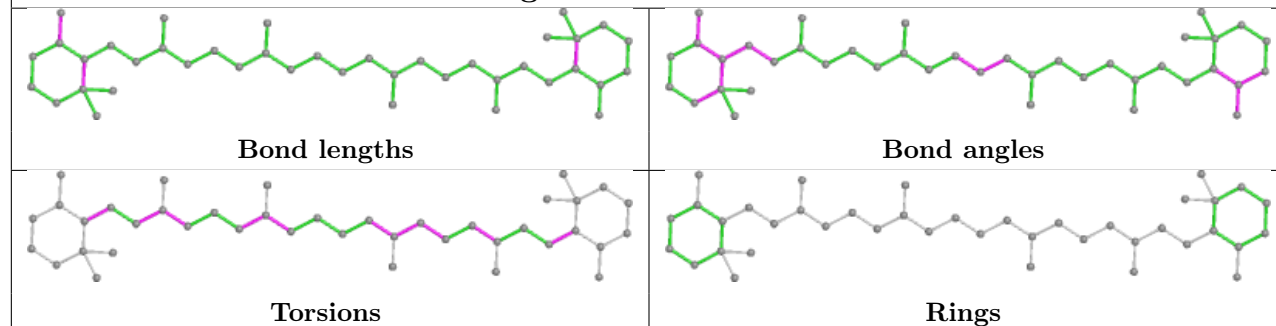
Ligand BCR K1 106



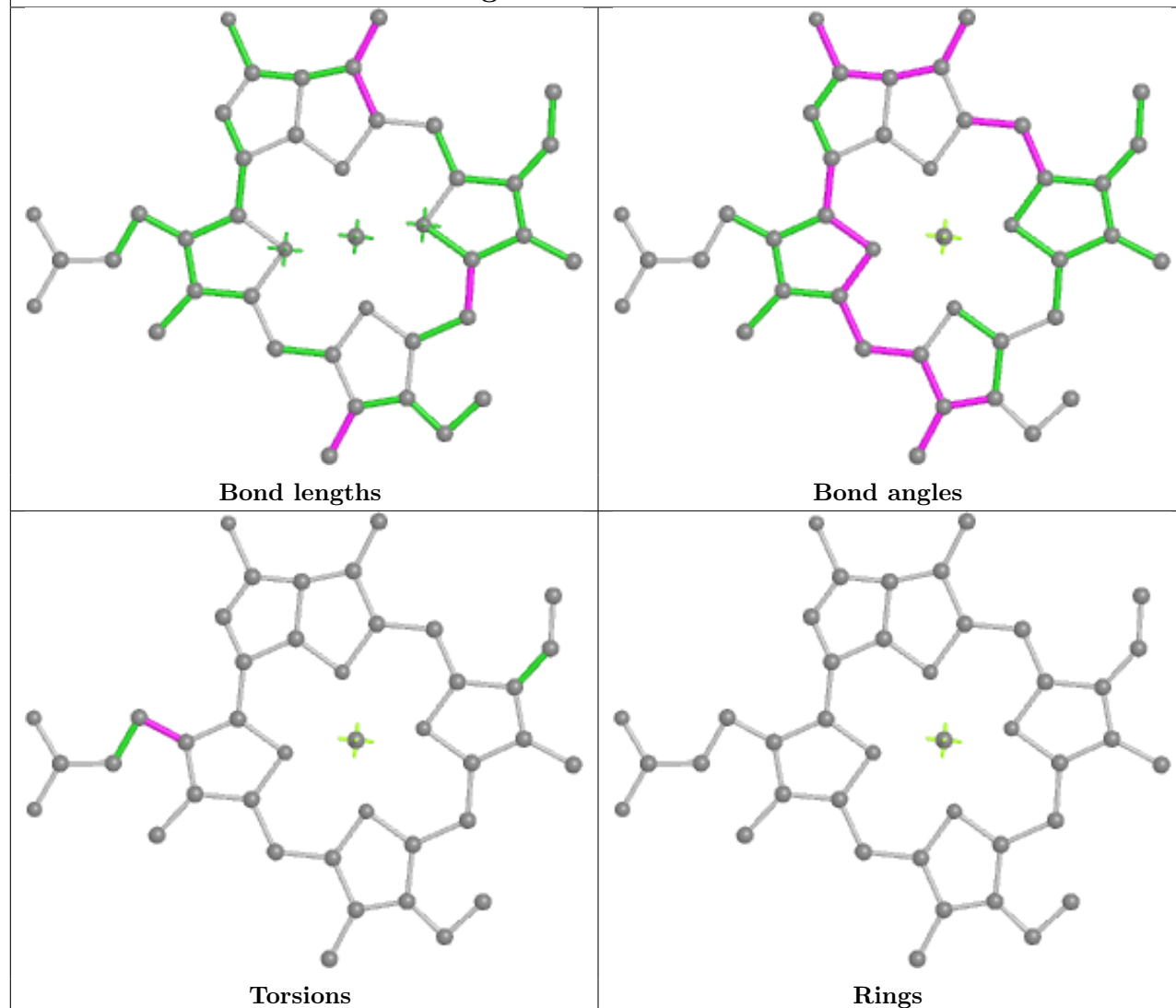
Ligand CLA K2 102



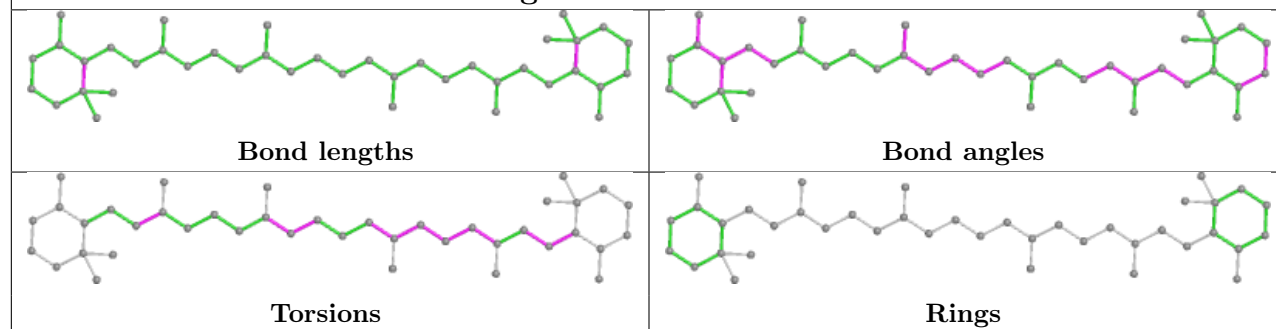
Ligand BCR K2 103



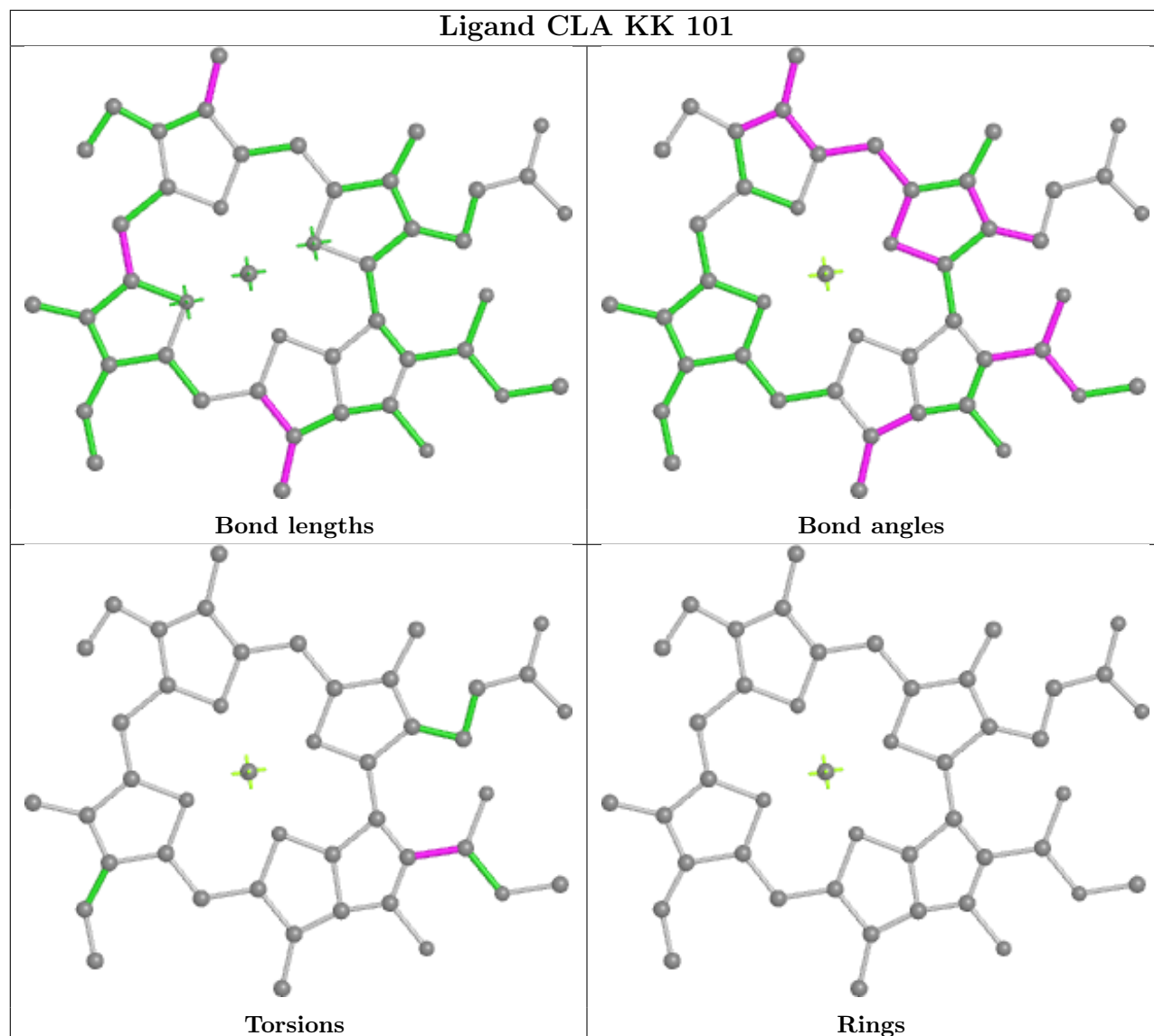
Ligand CLA K2 104



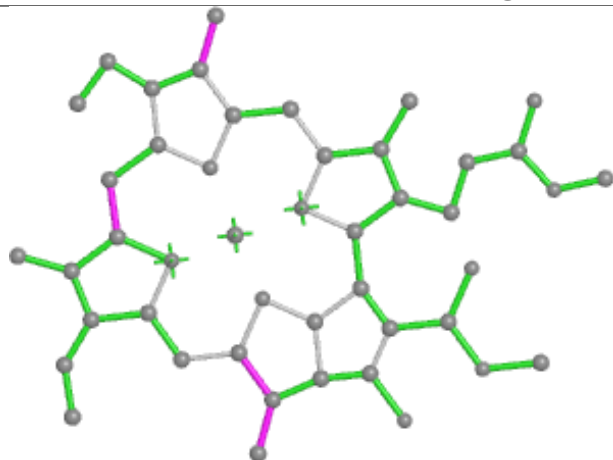
Ligand BCR K2 105



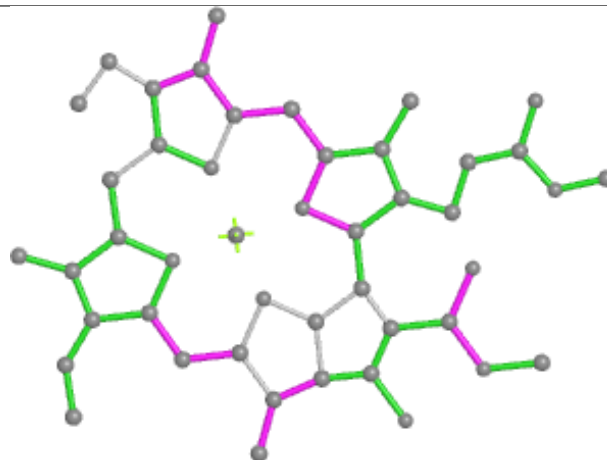
Ligand CLA KK 101



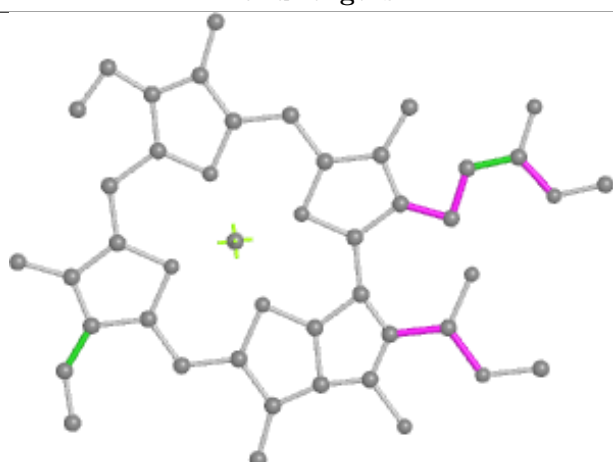
Ligand CLA KK 102



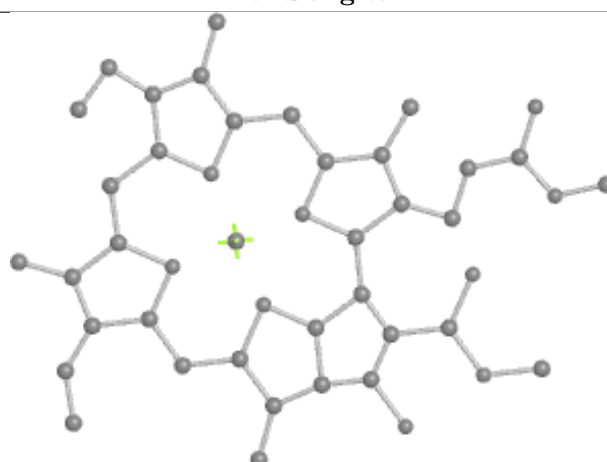
Bond lengths



Bond angles

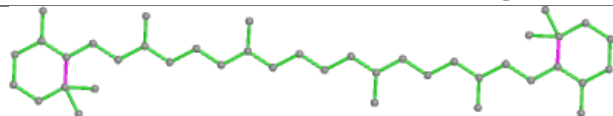


Torsions

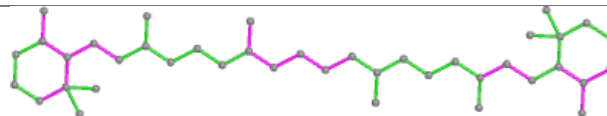


Rings

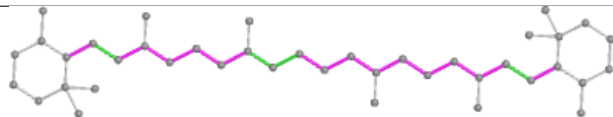
Ligand BCR KK 103



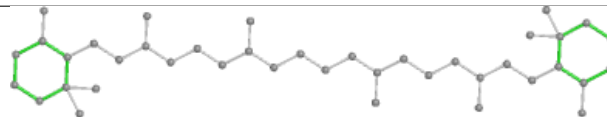
Bond lengths



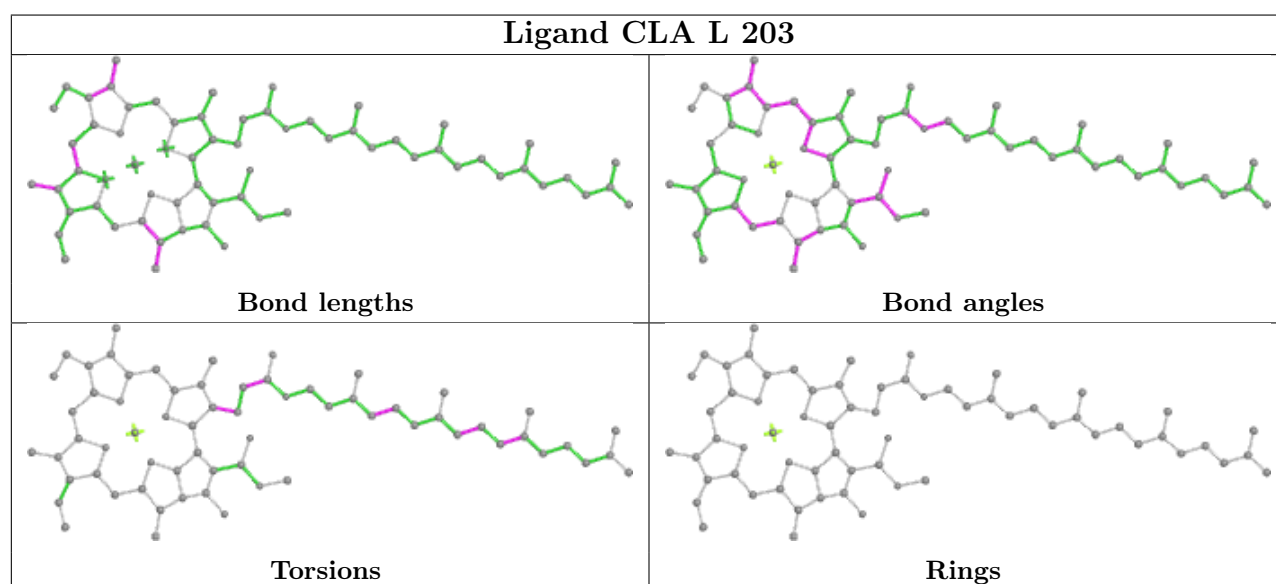
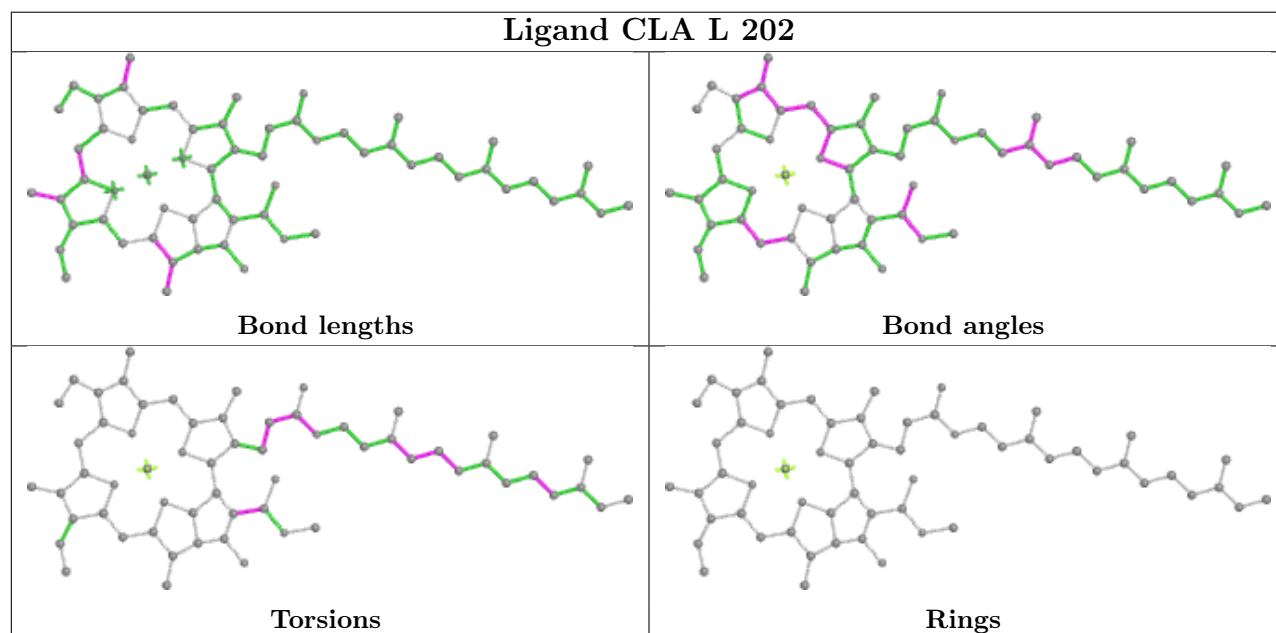
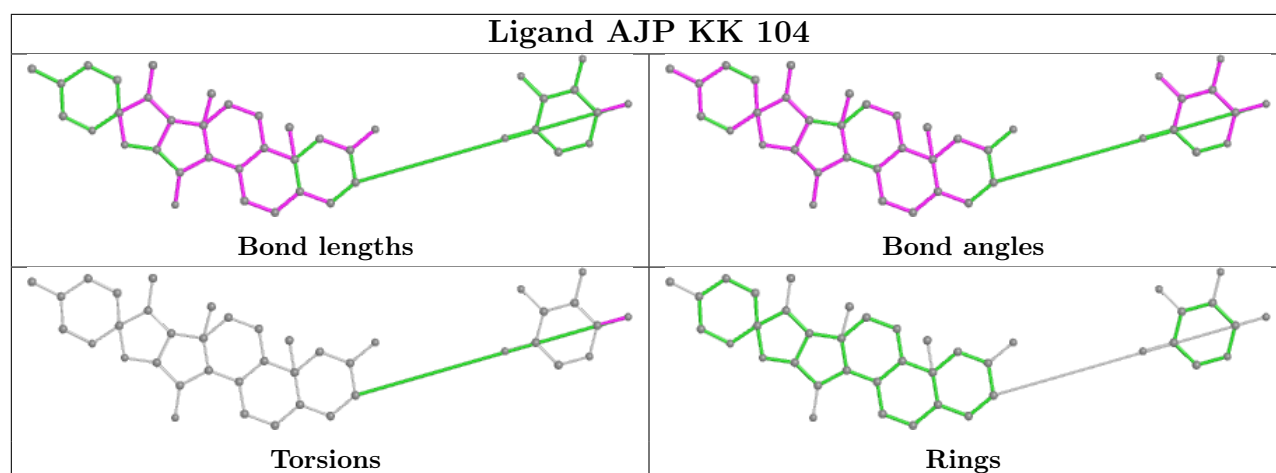
Bond angles

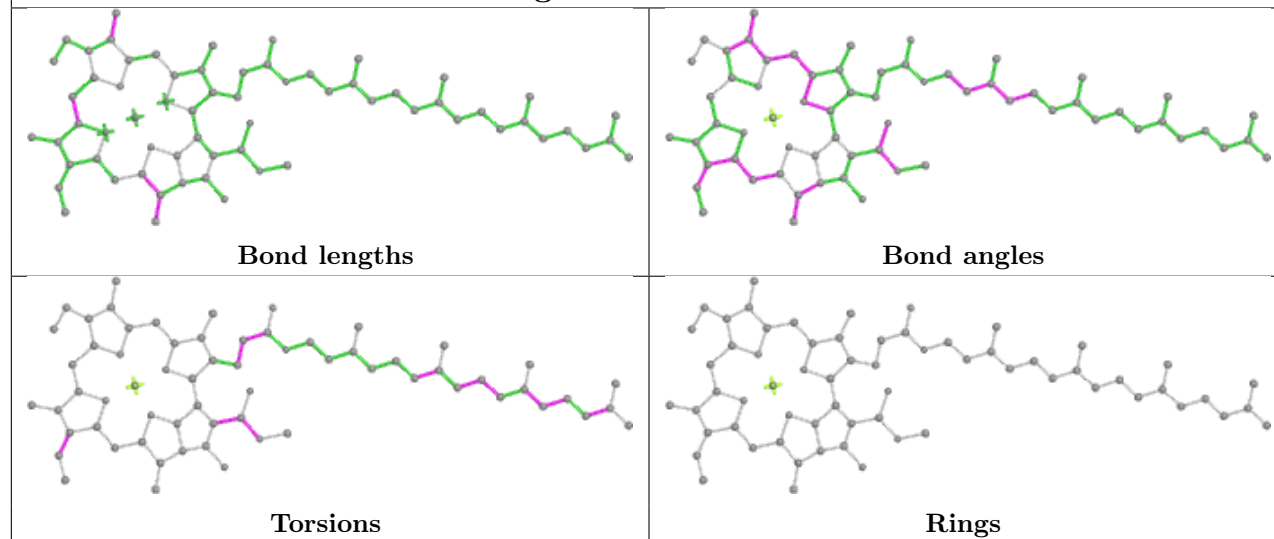
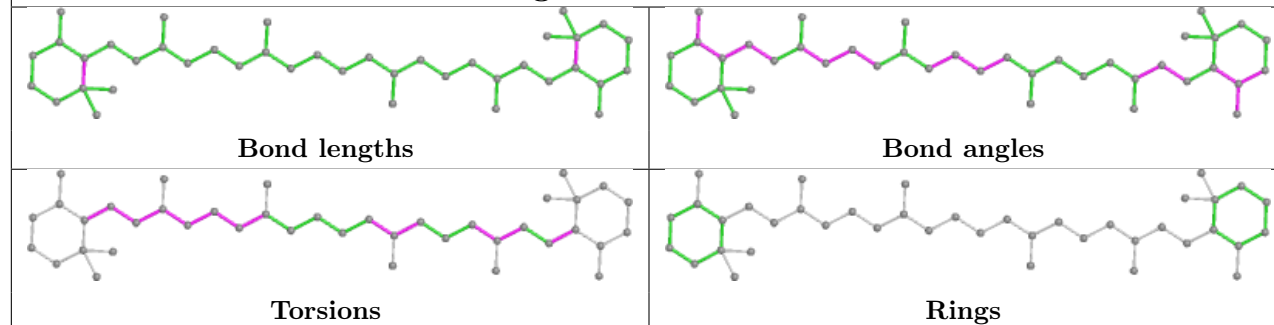


Torsions

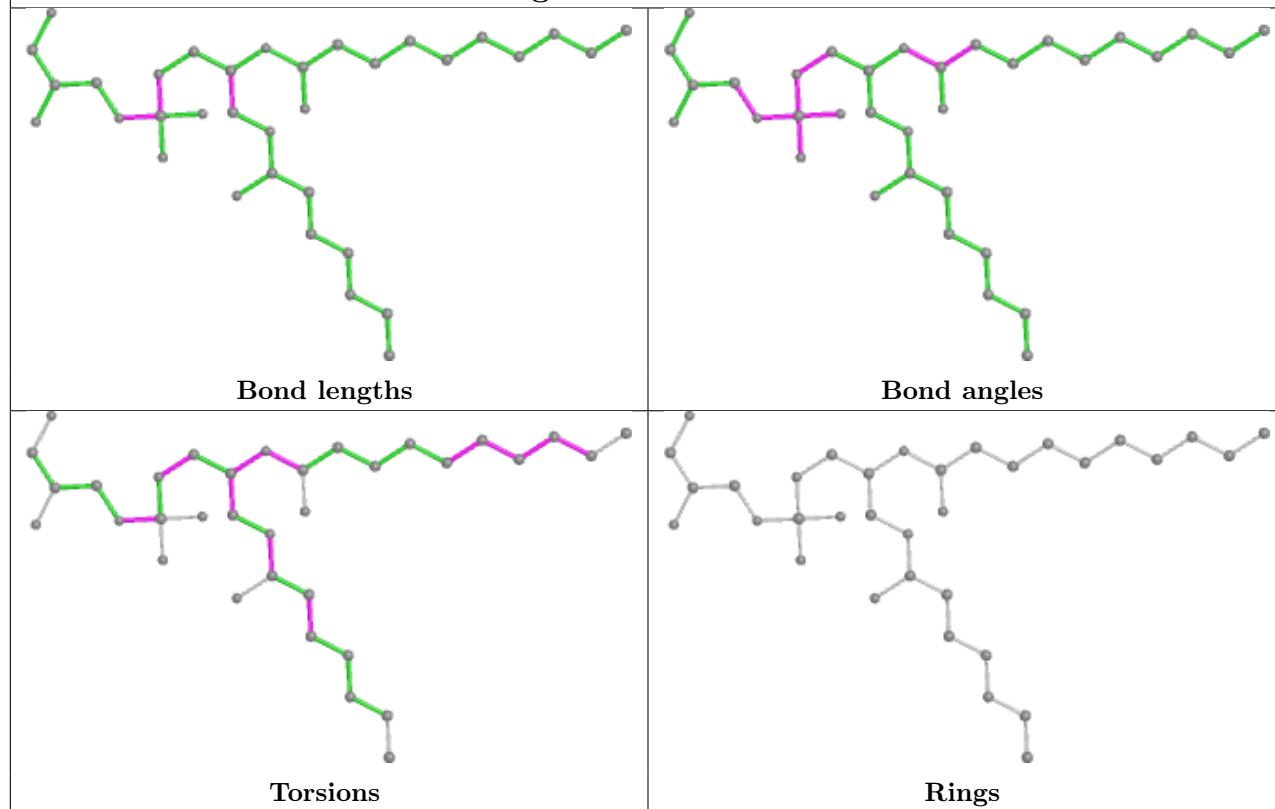


Rings

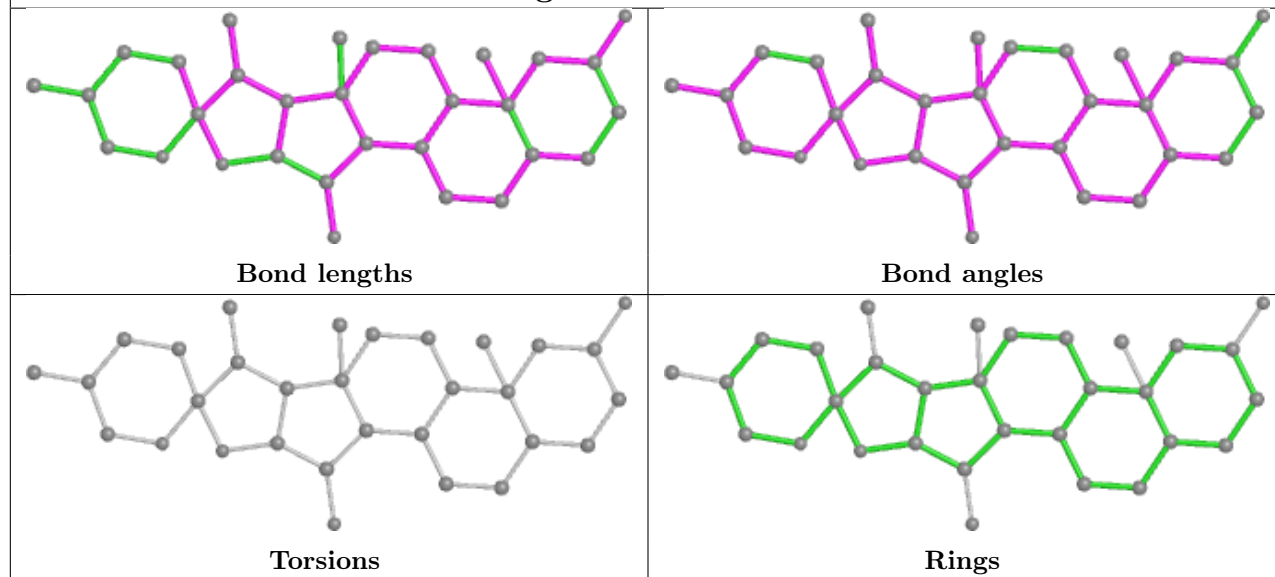


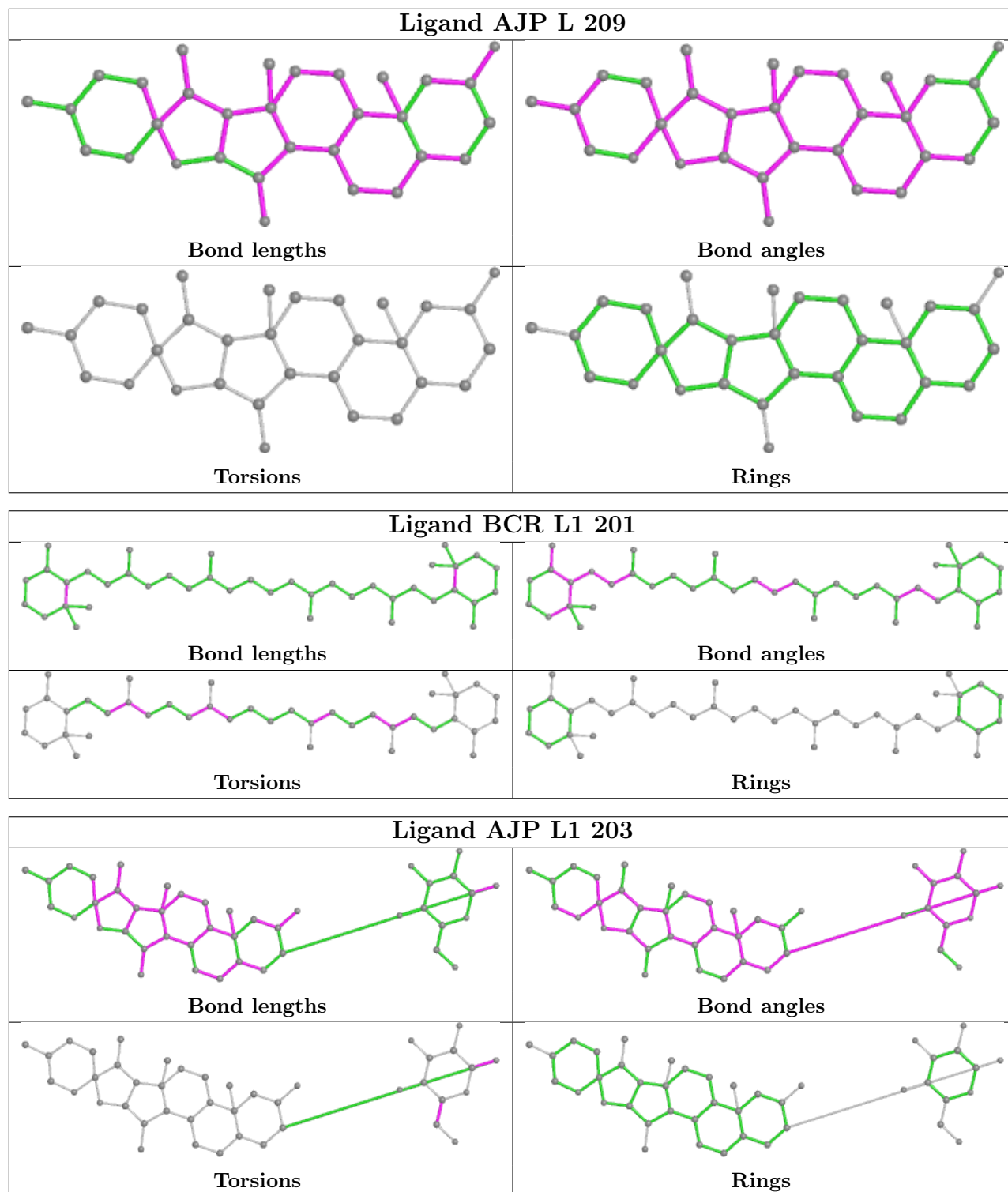
Ligand CLA L 204**Ligand BCR L 205****Ligand BCR L 206**

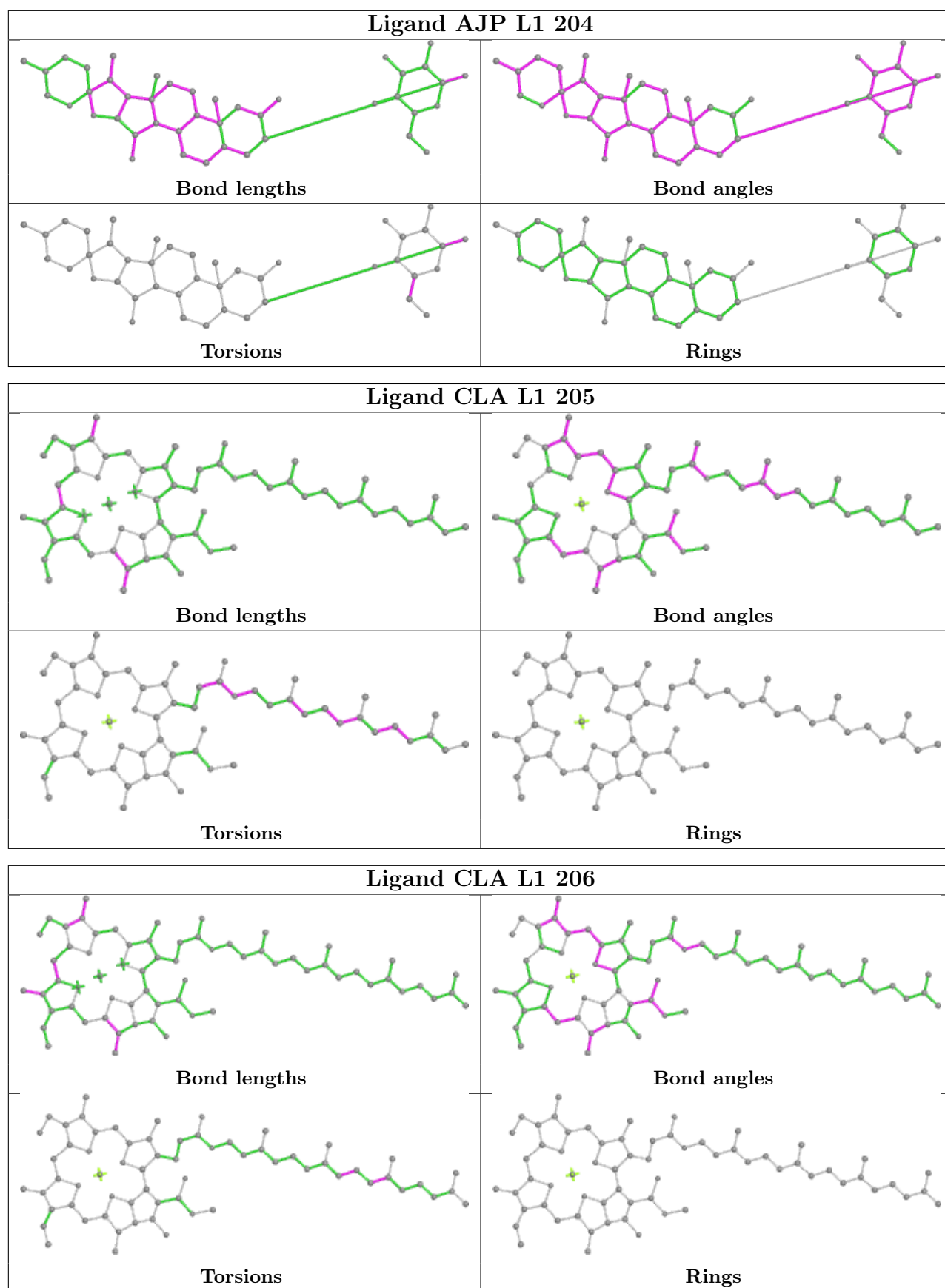
Ligand LHG L 207

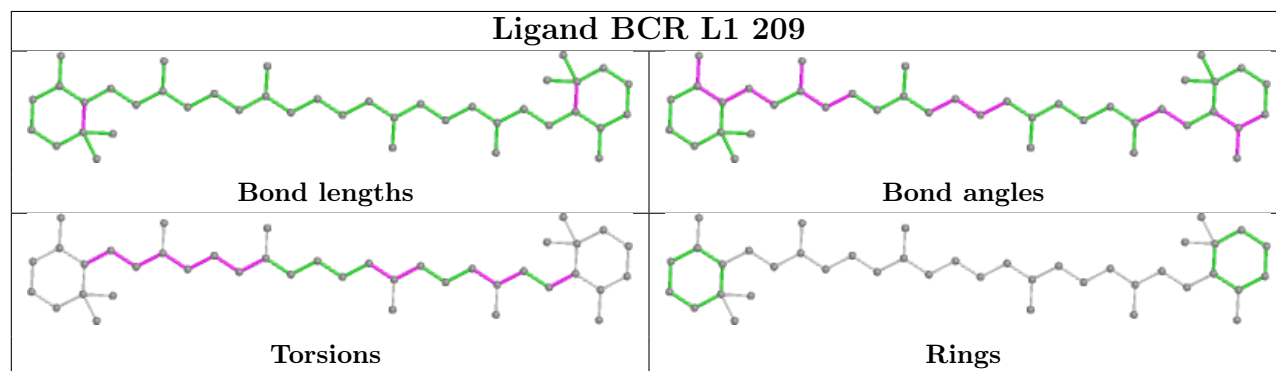
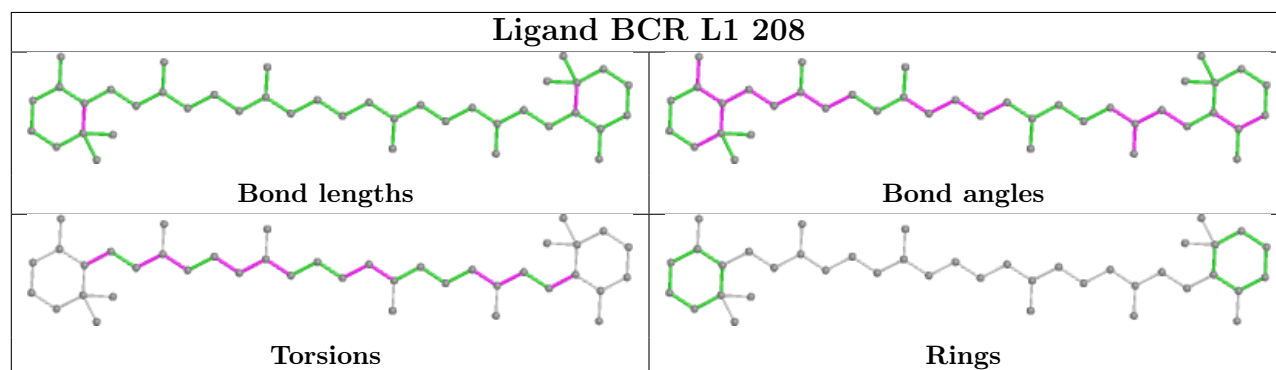
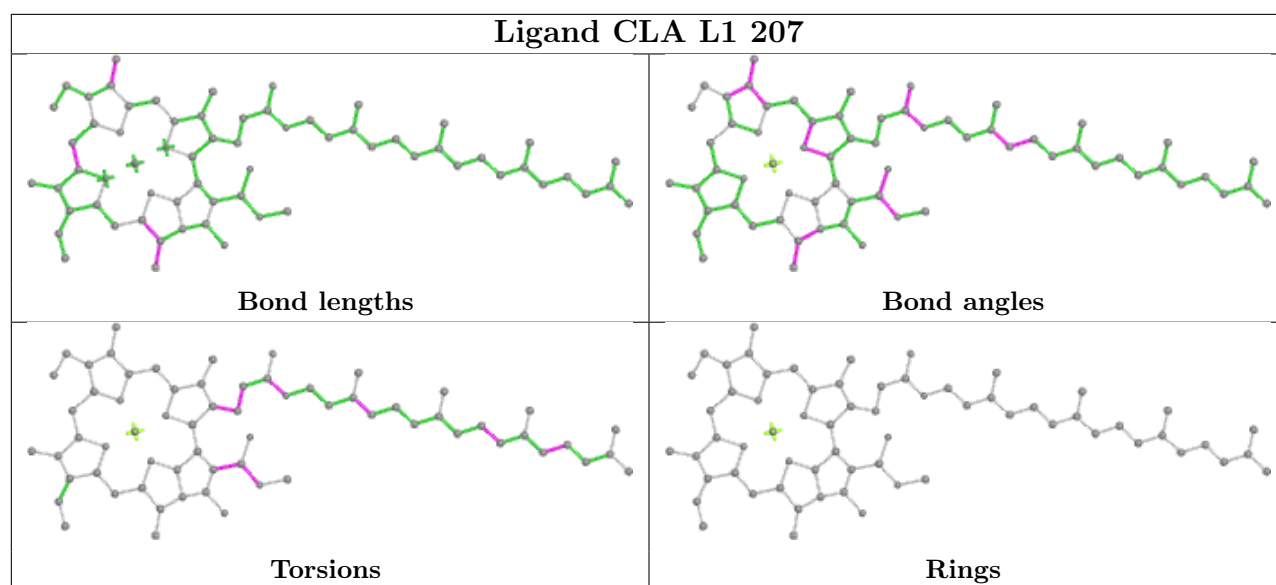


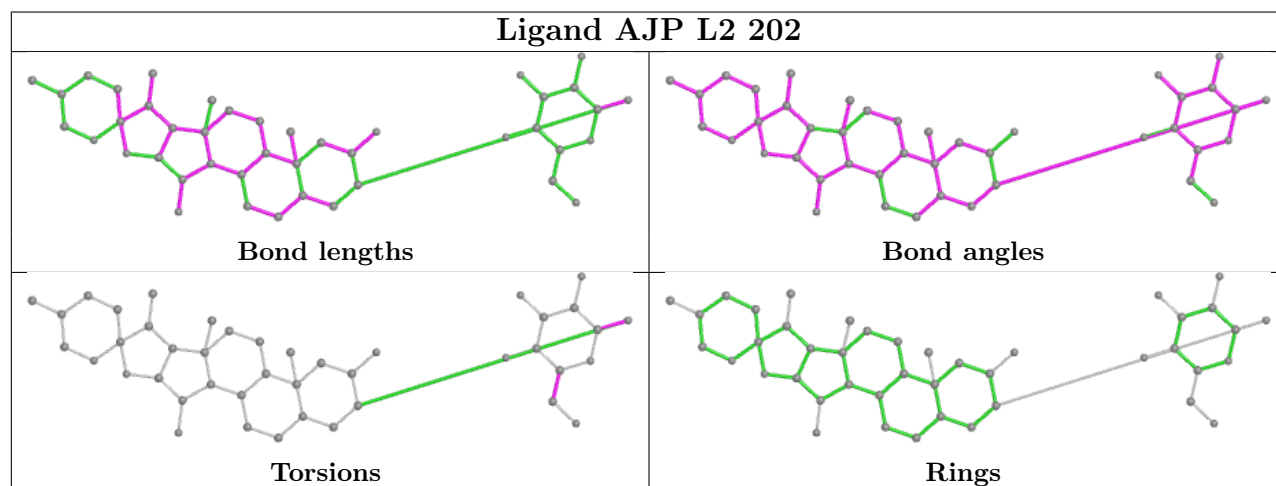
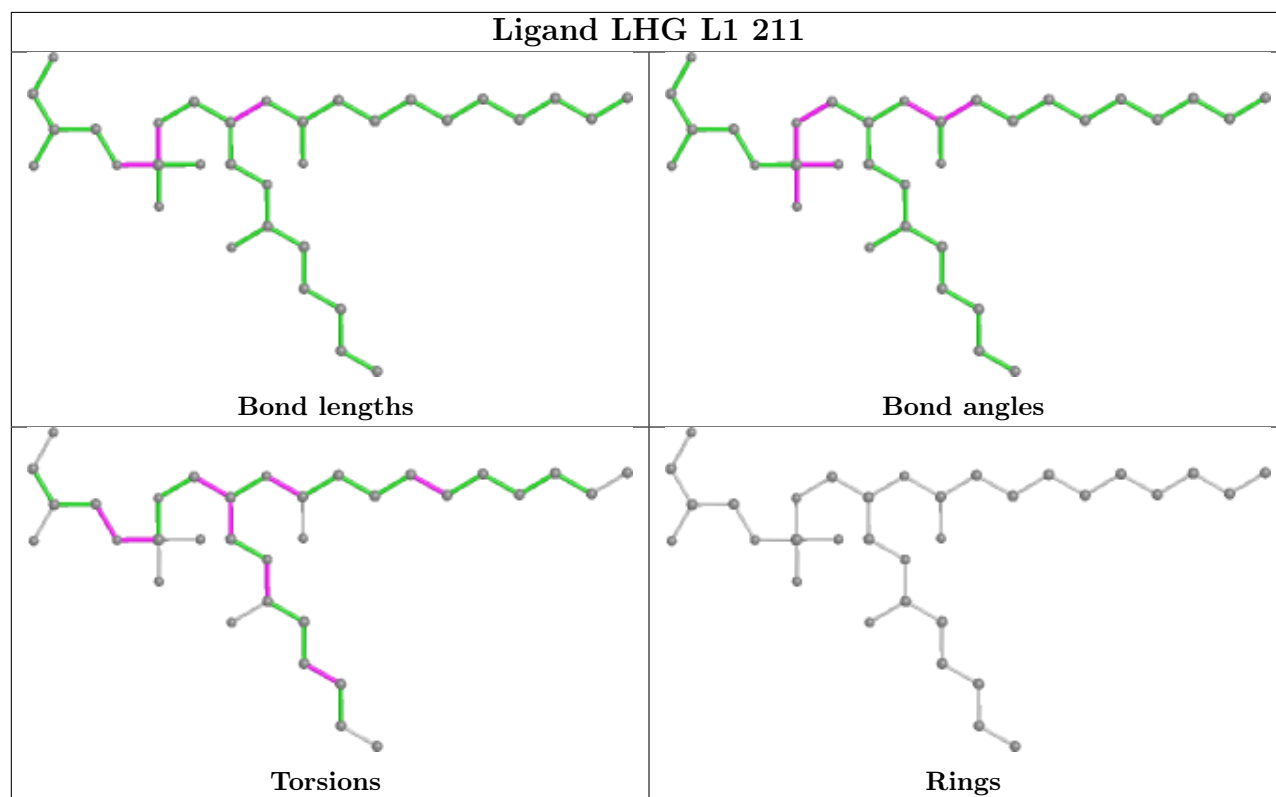
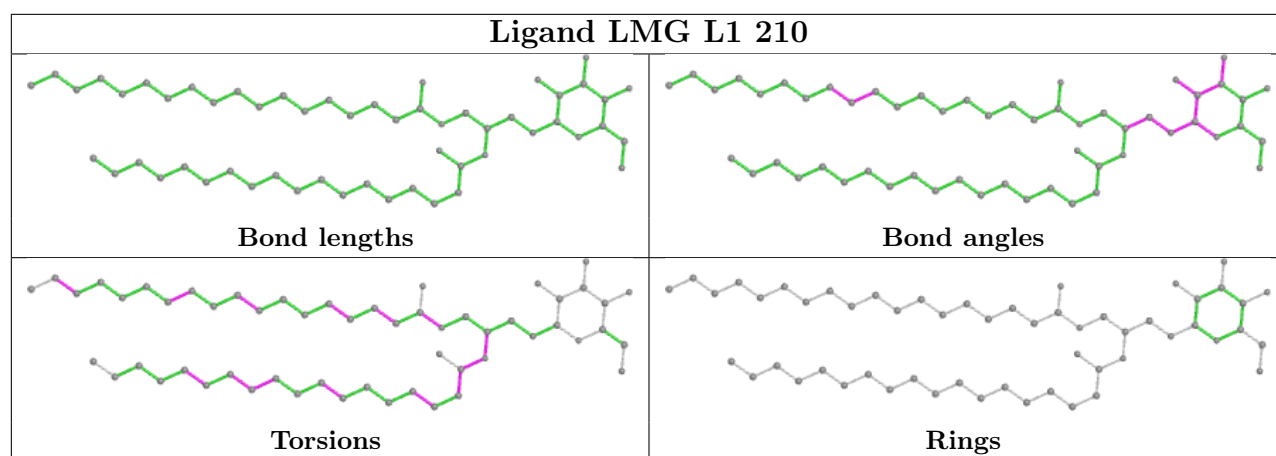
Ligand AJP L 208

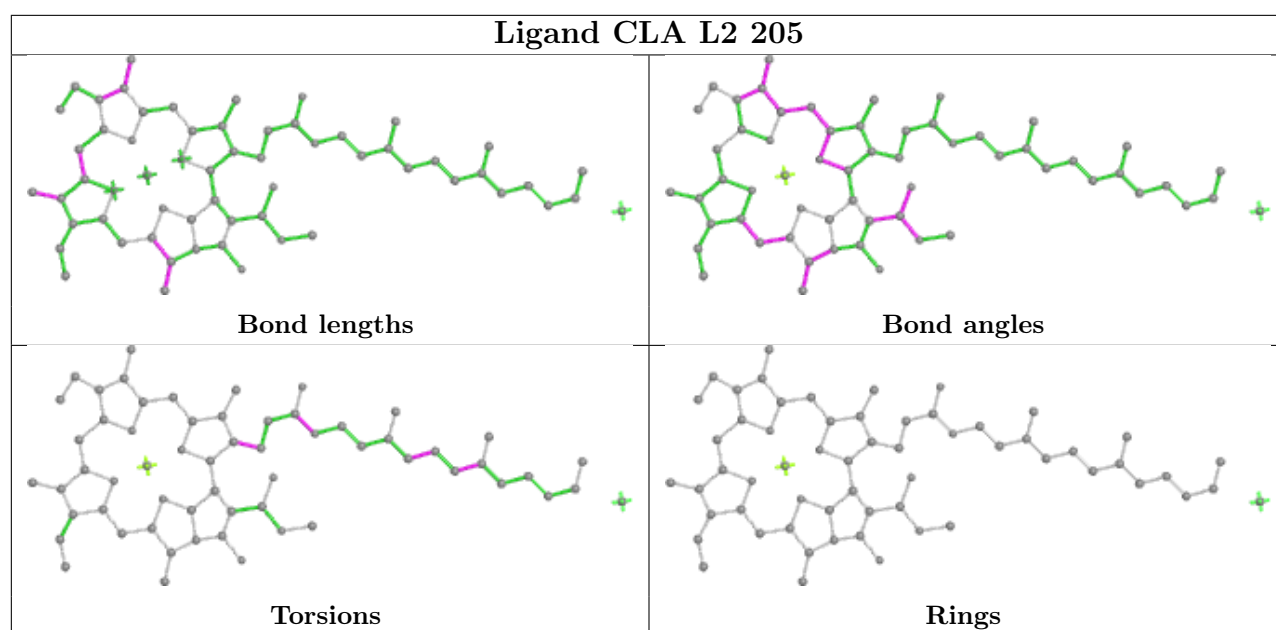
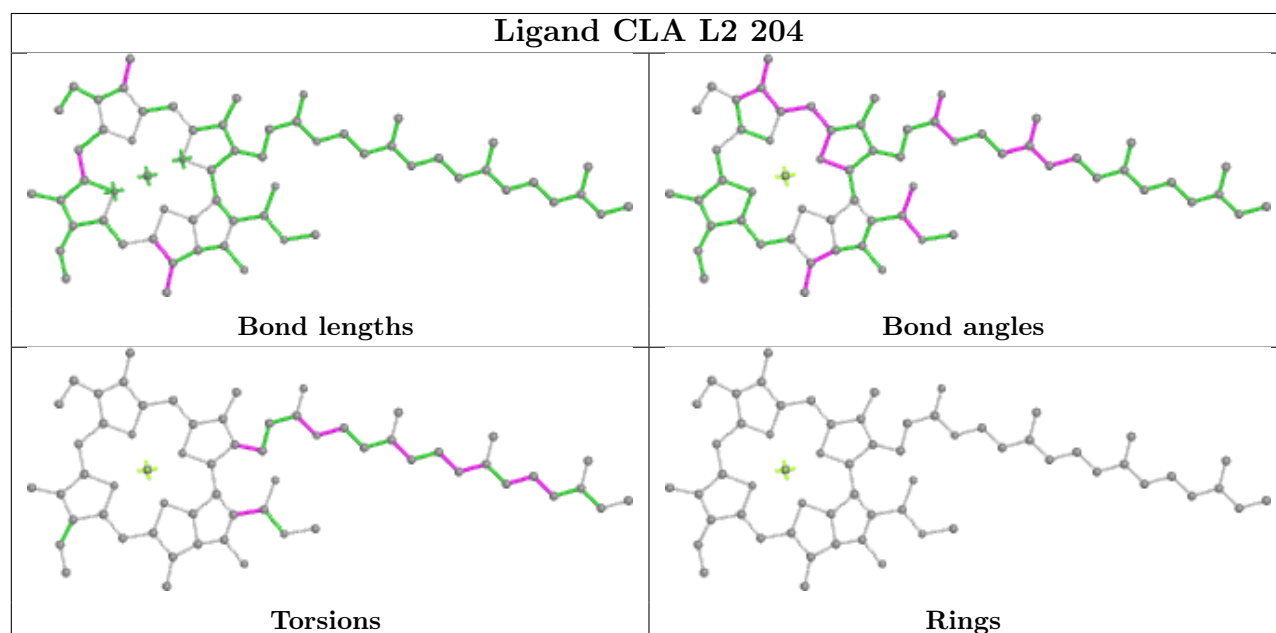
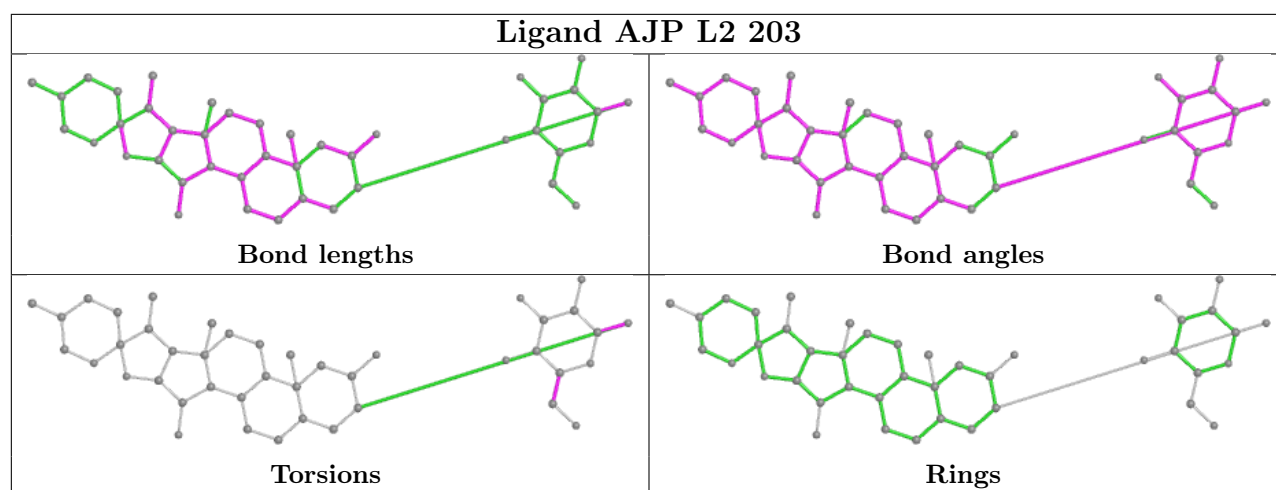


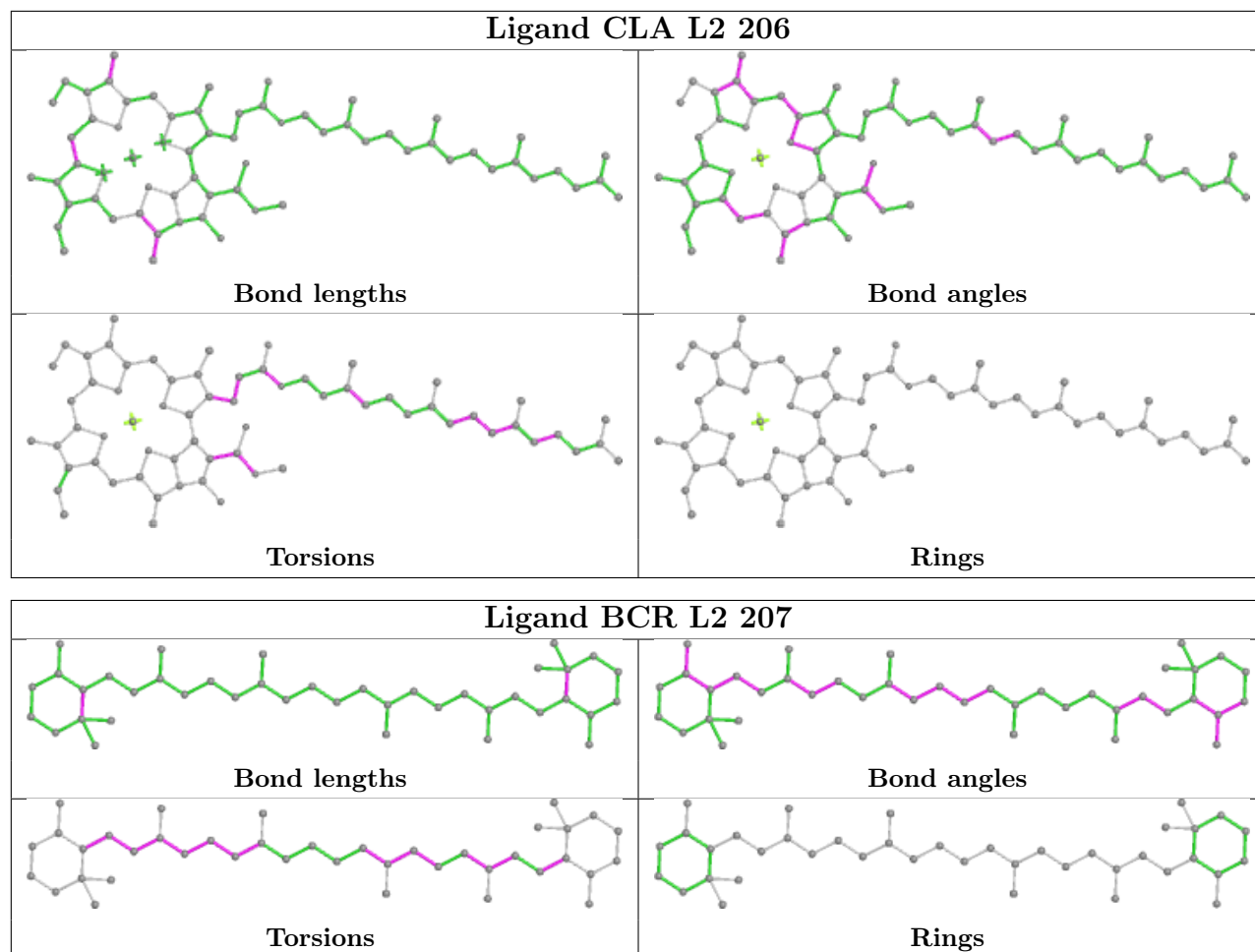


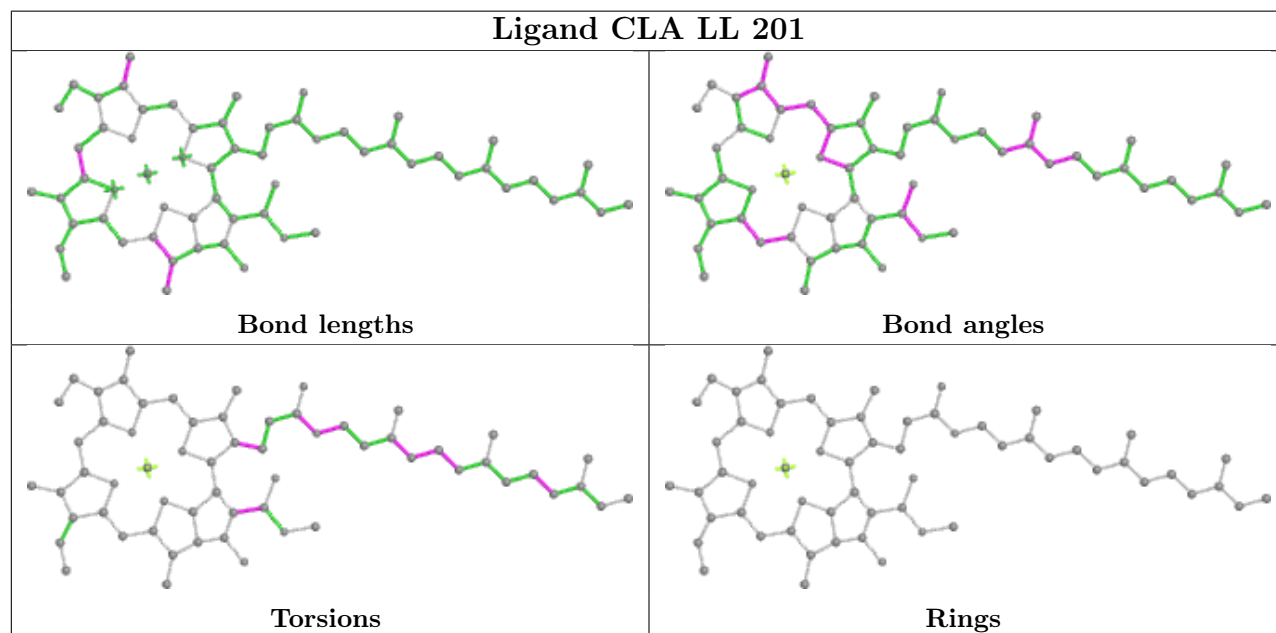
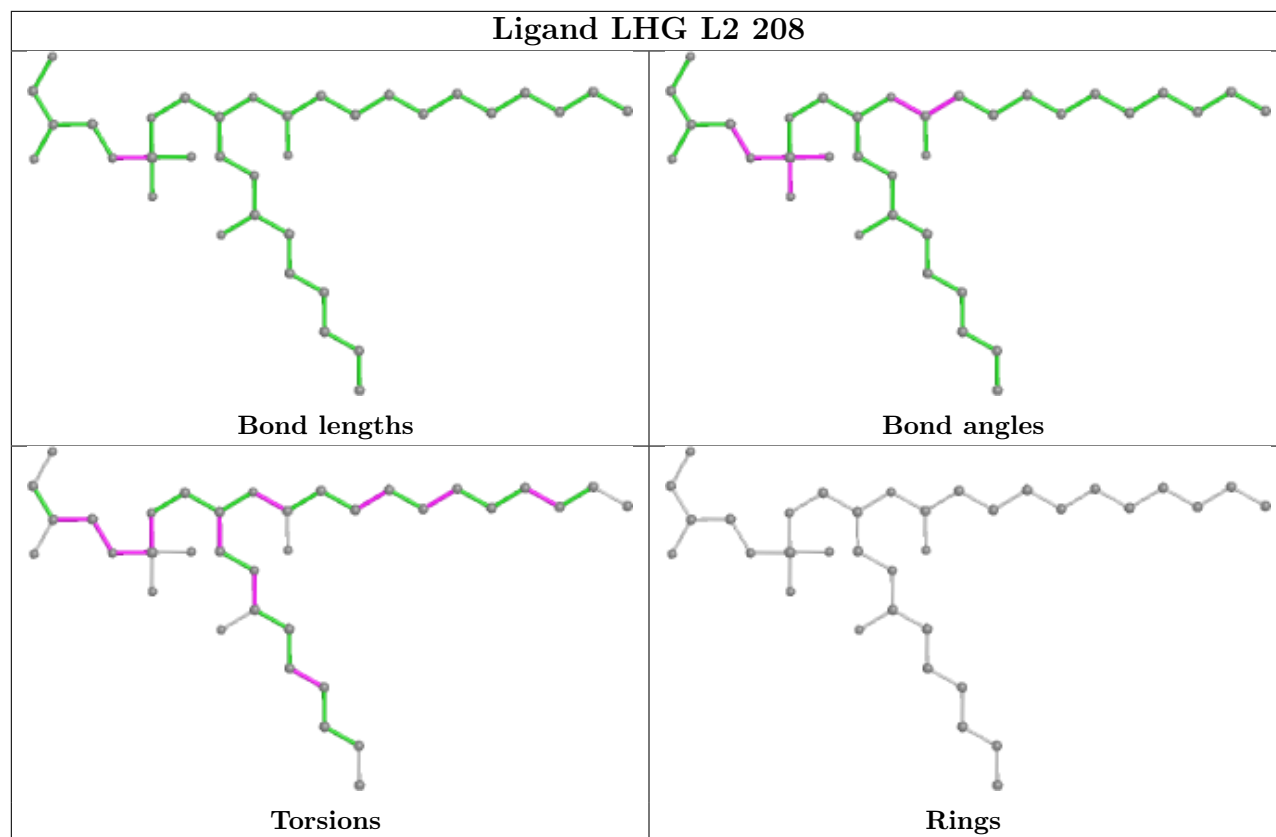




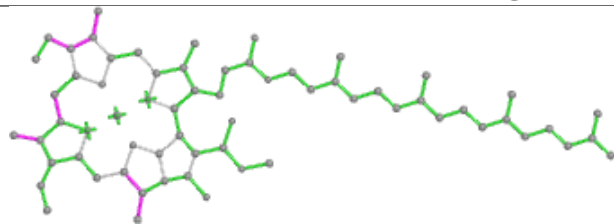




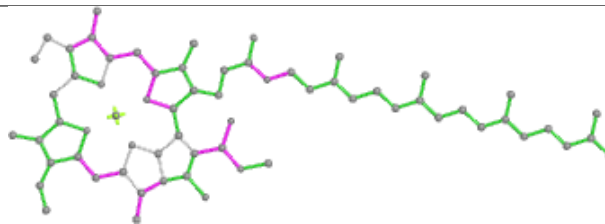




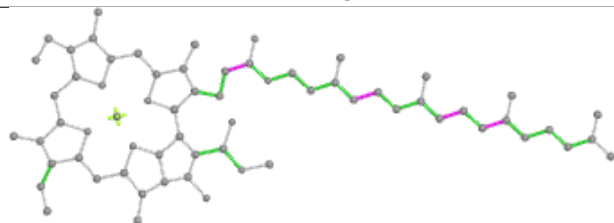
Ligand CLA LL 202



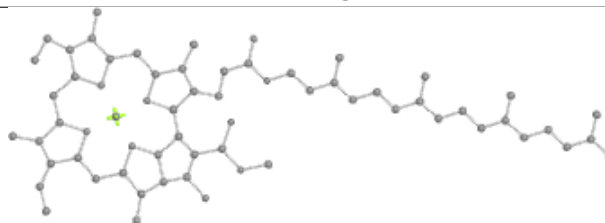
Bond lengths



Bond angles

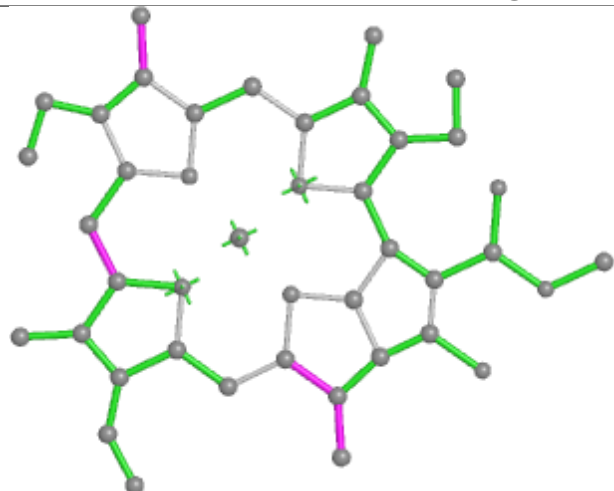


Torsions

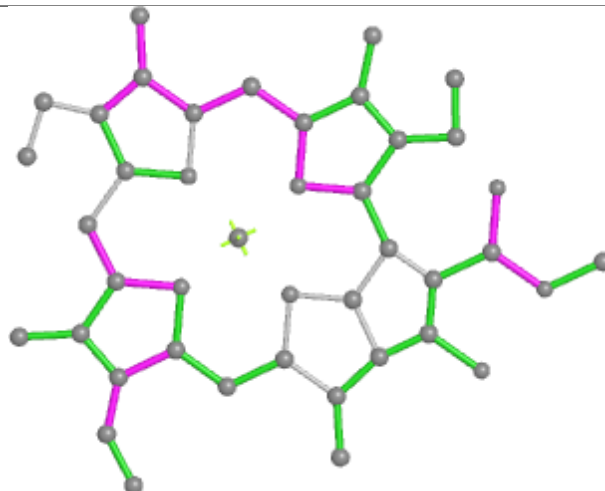


Rings

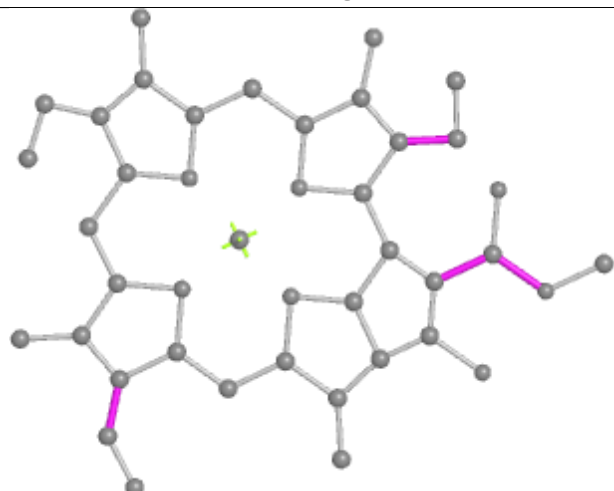
Ligand CLA LL 203



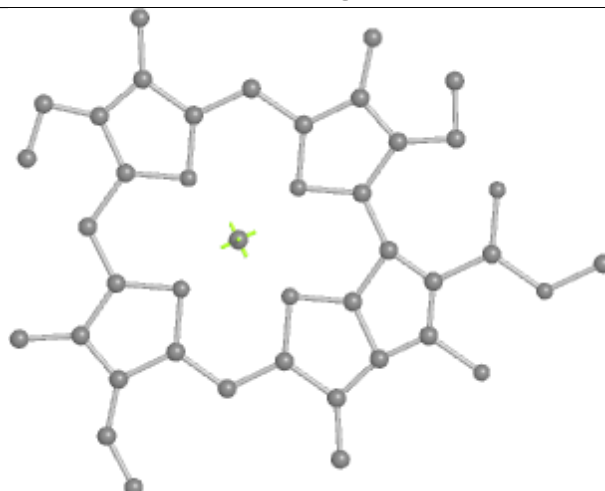
Bond lengths



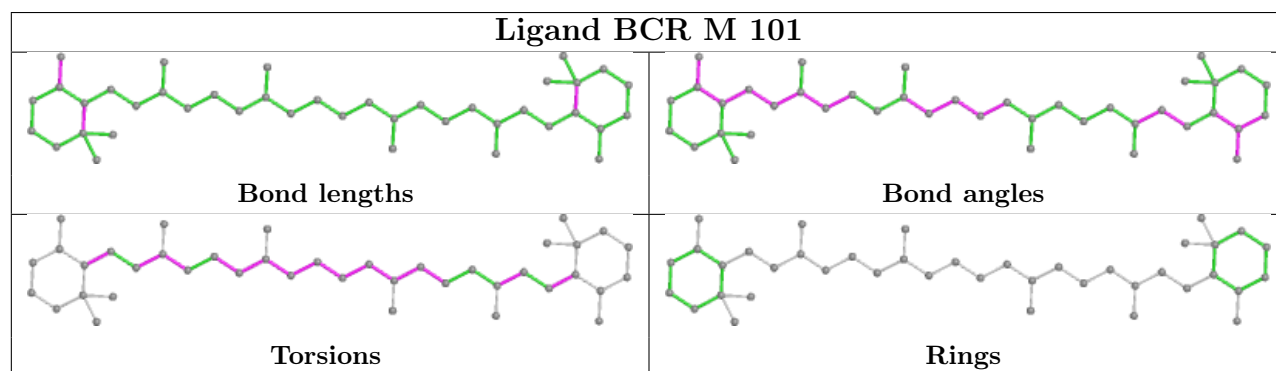
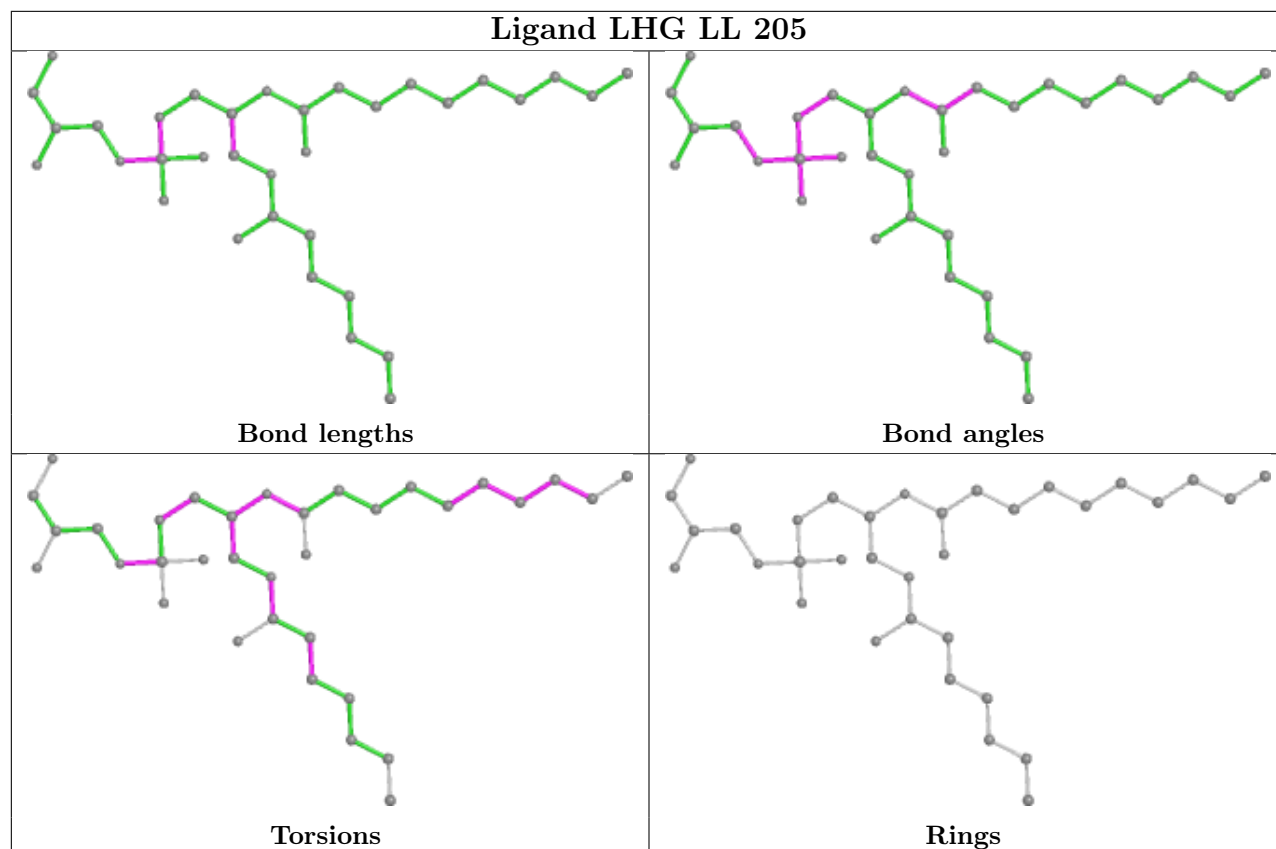
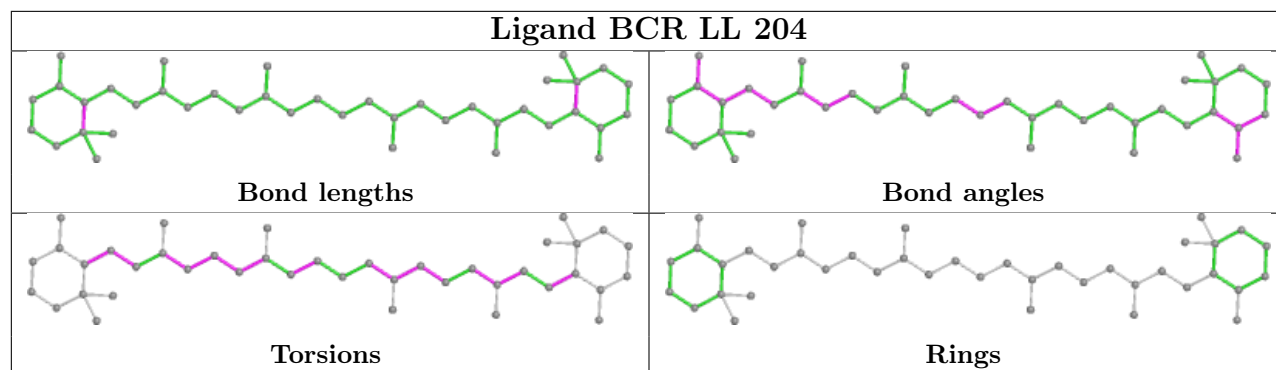
Bond angles

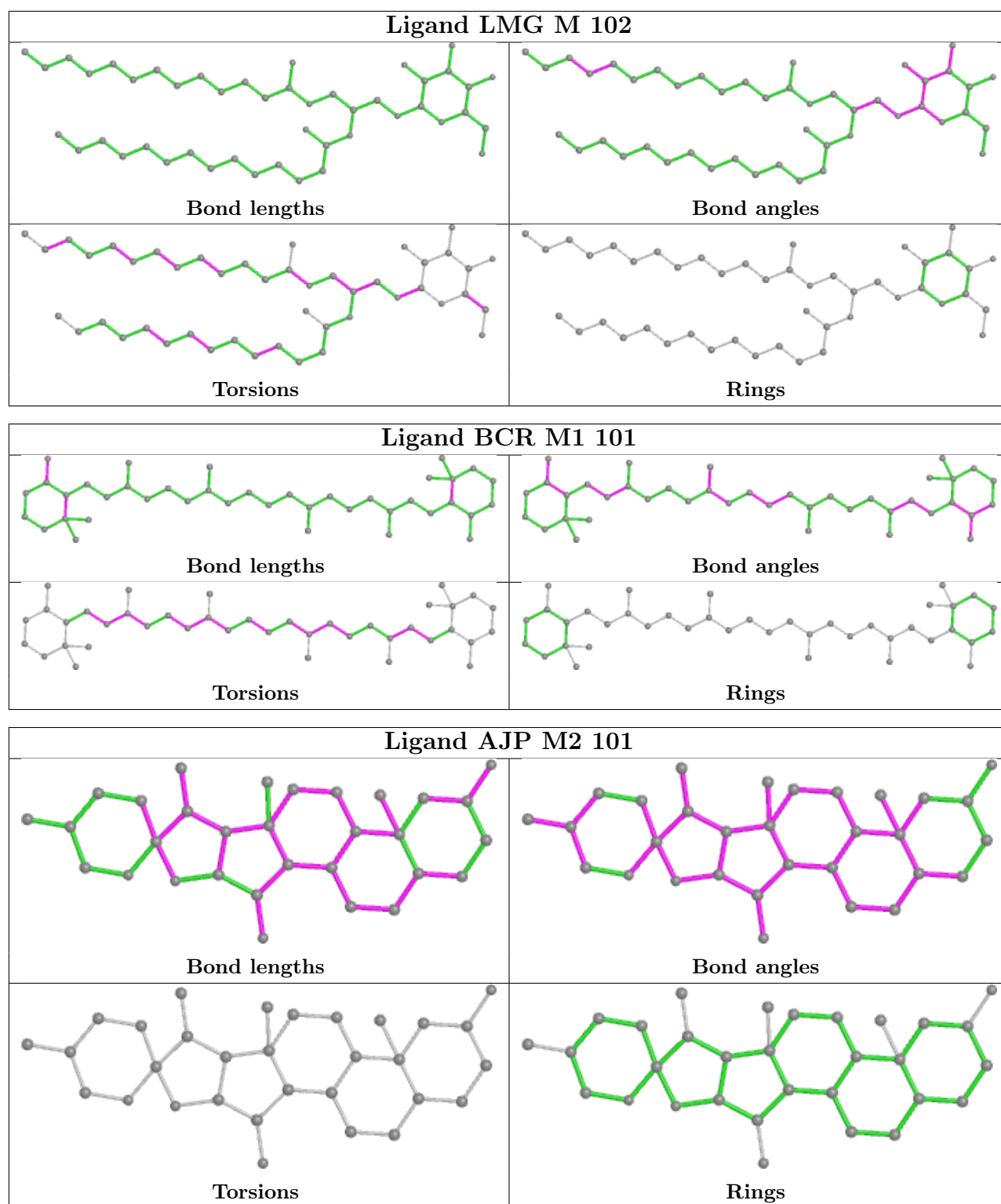


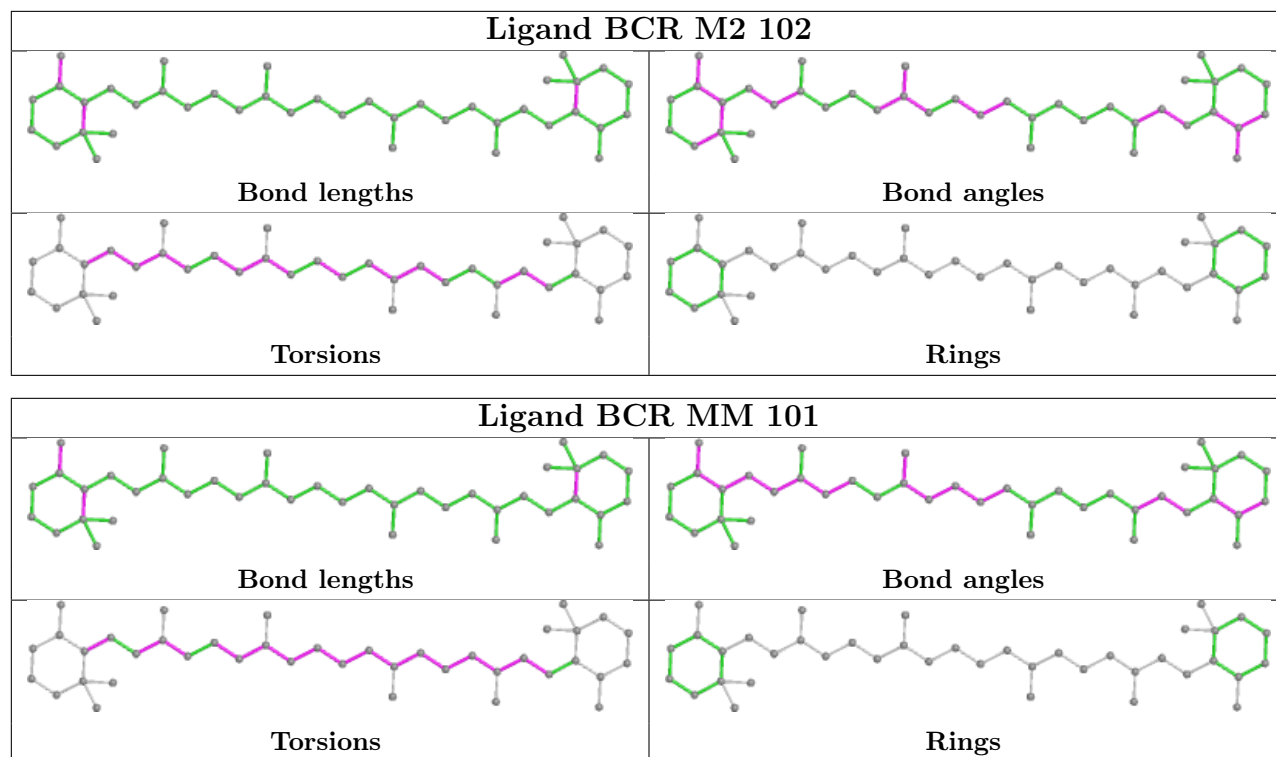
Torsions



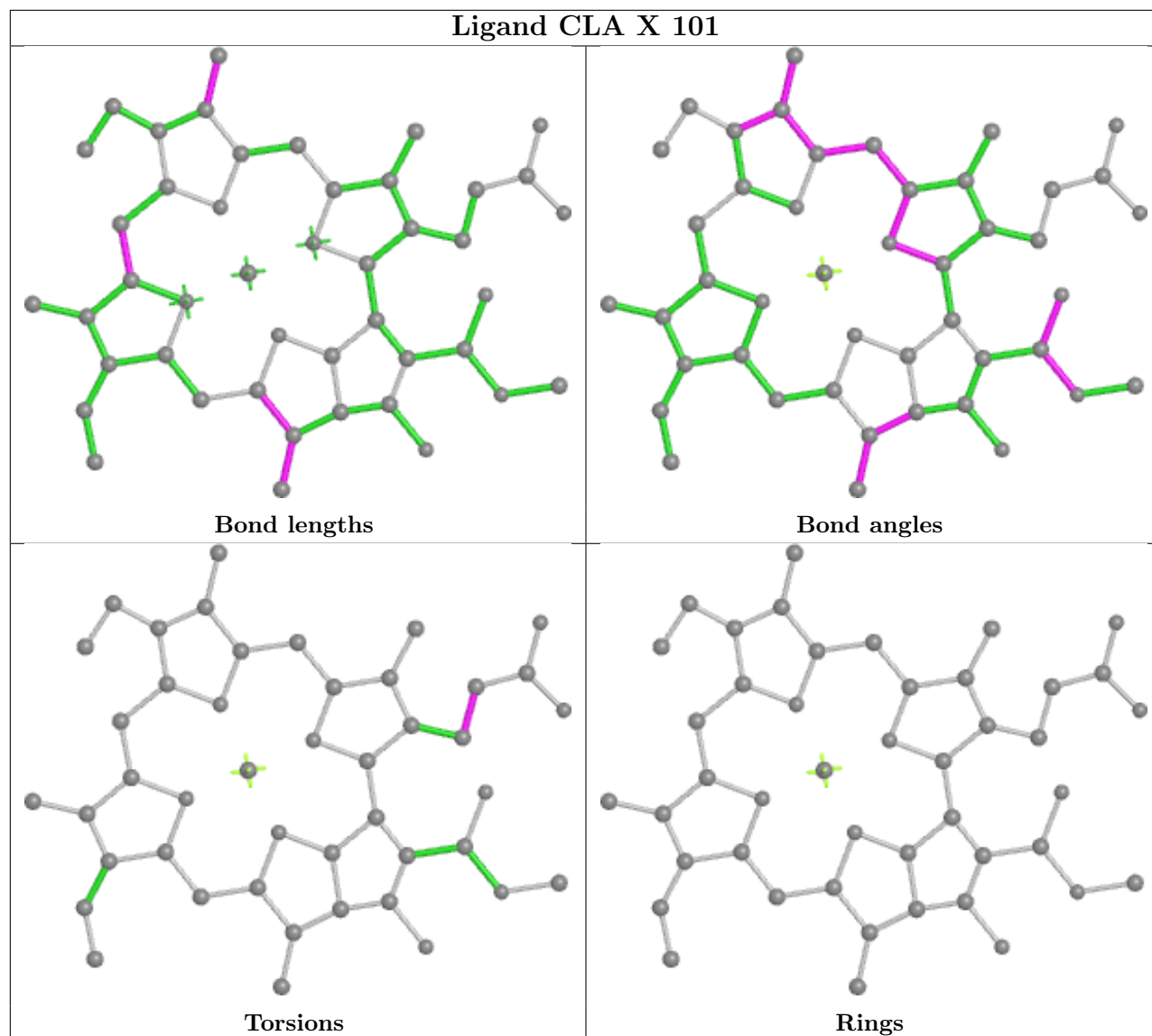
Rings

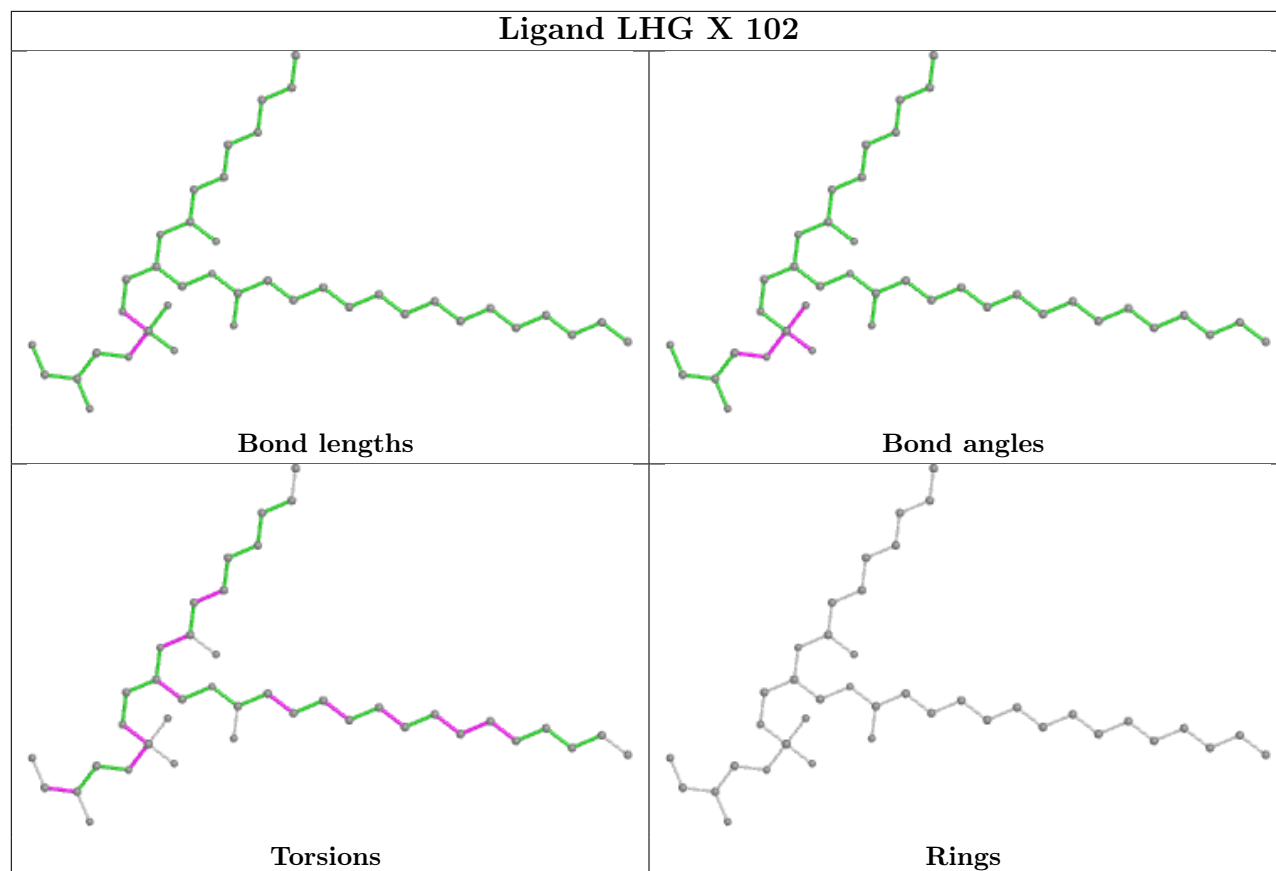




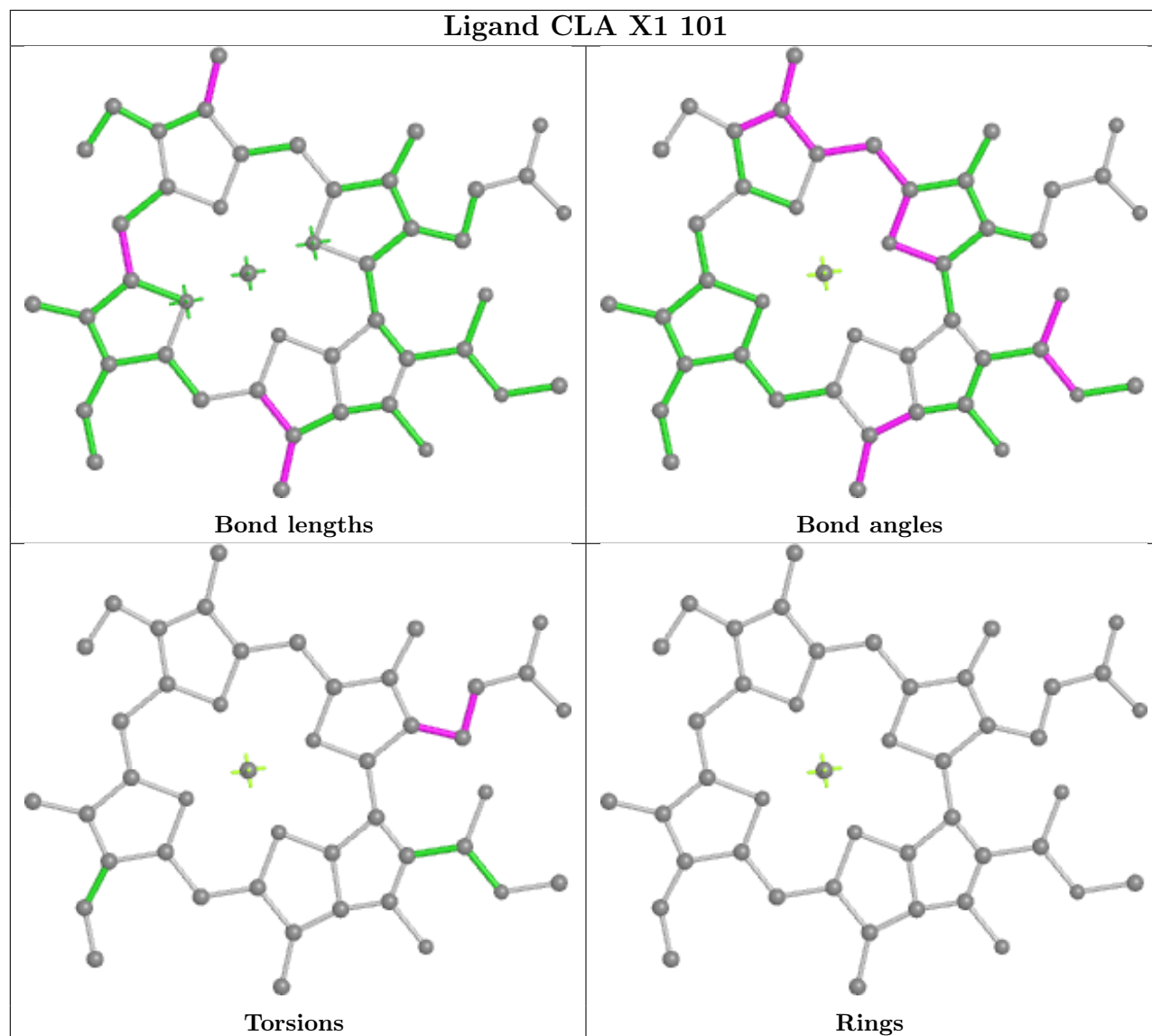


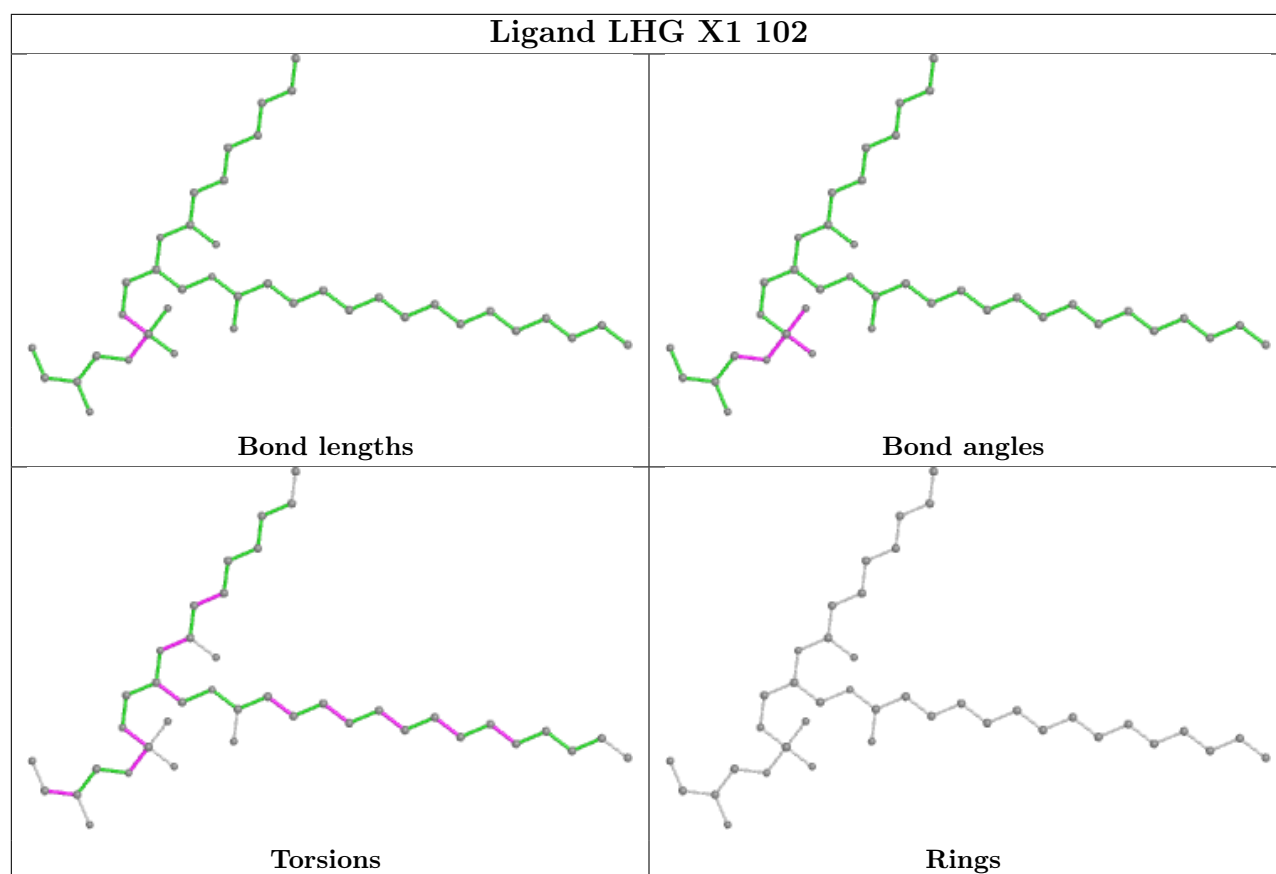
Ligand CLA X 101

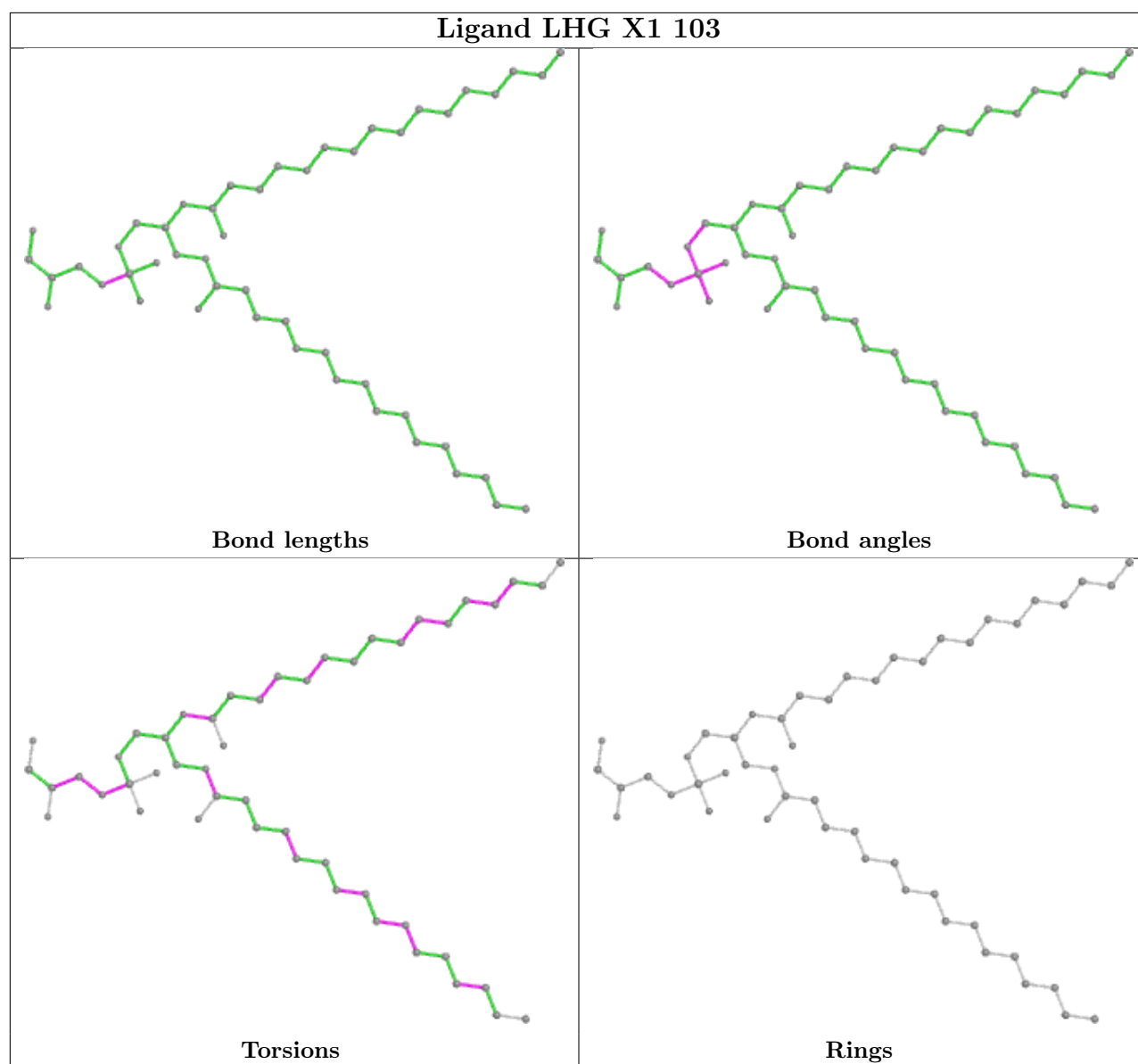




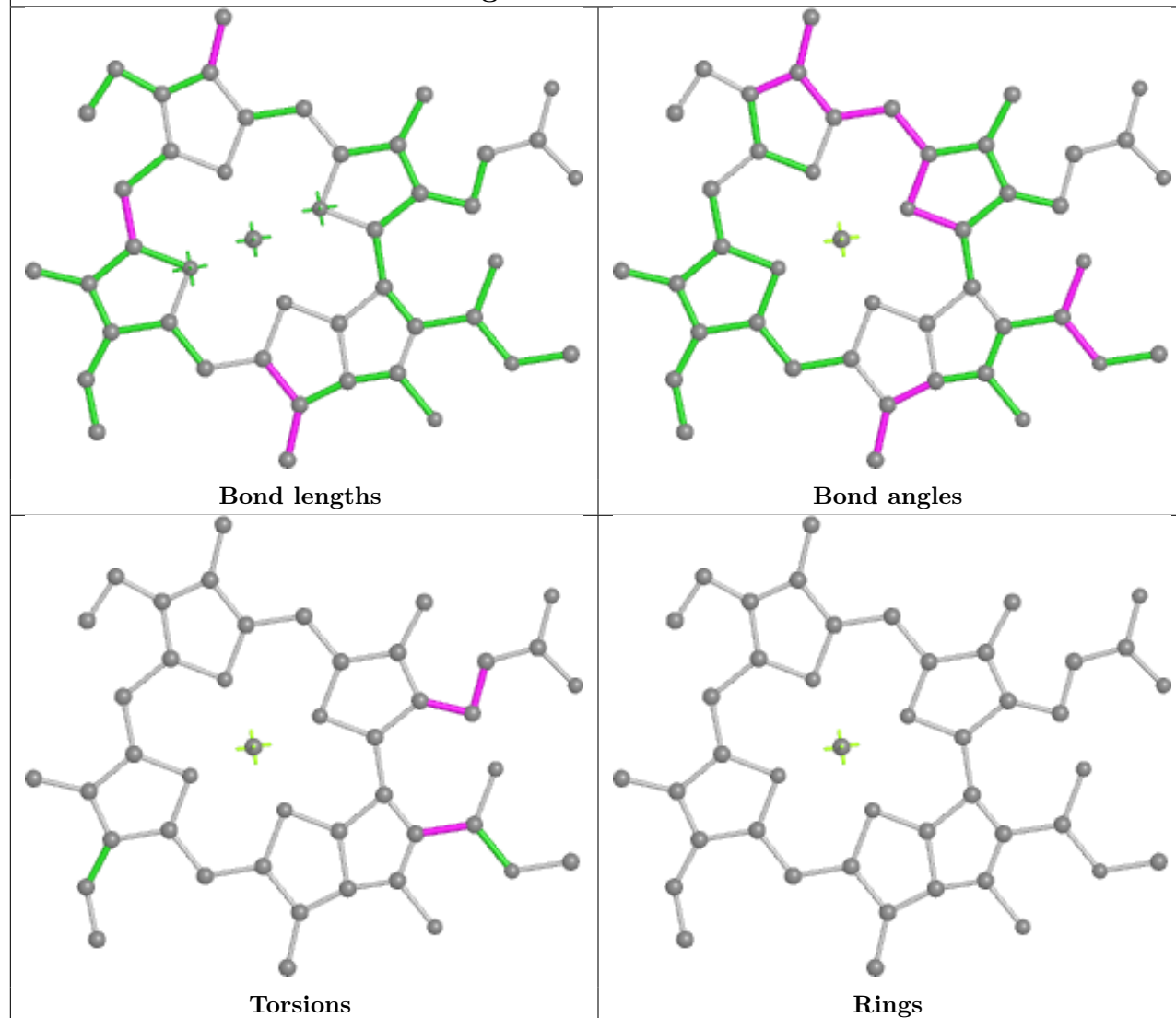
Ligand CLA X1 101

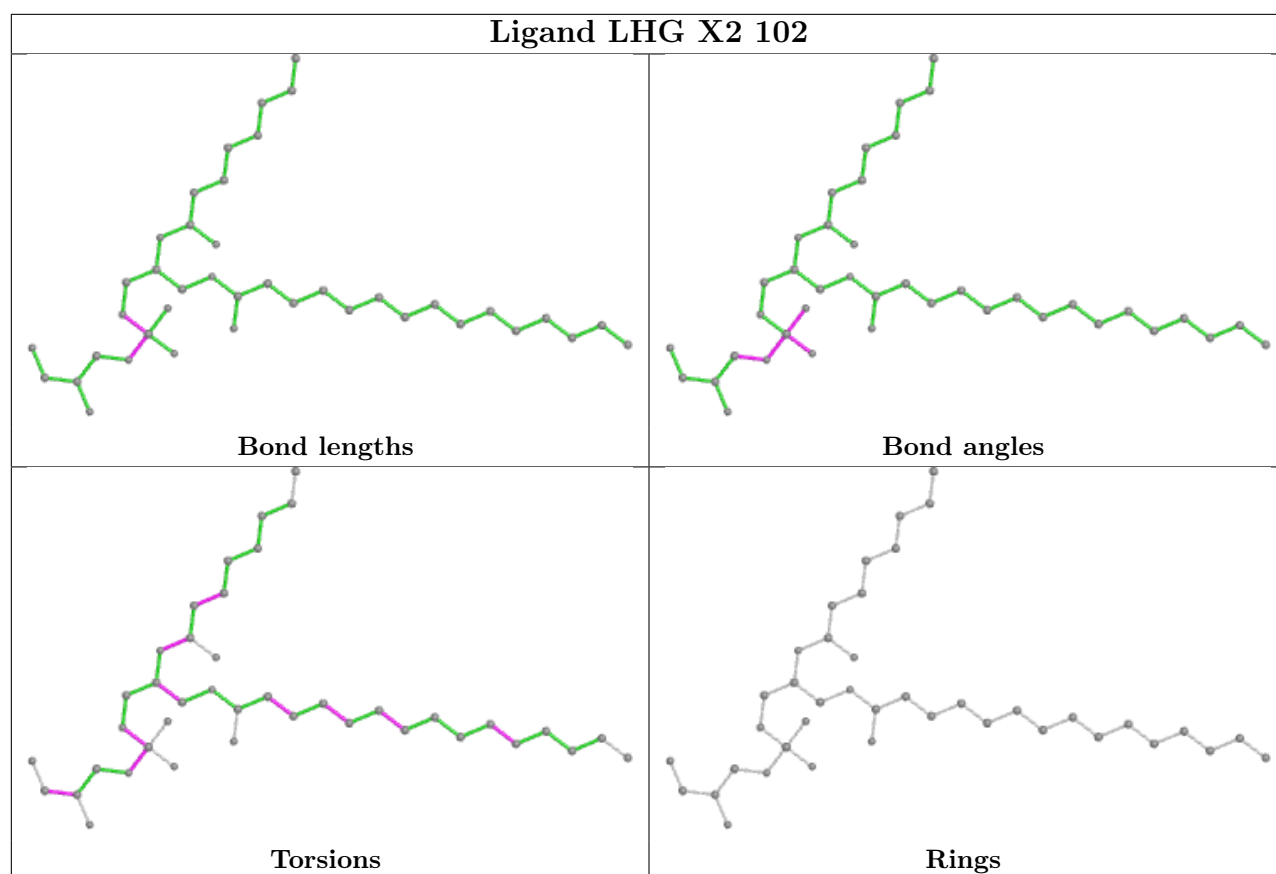


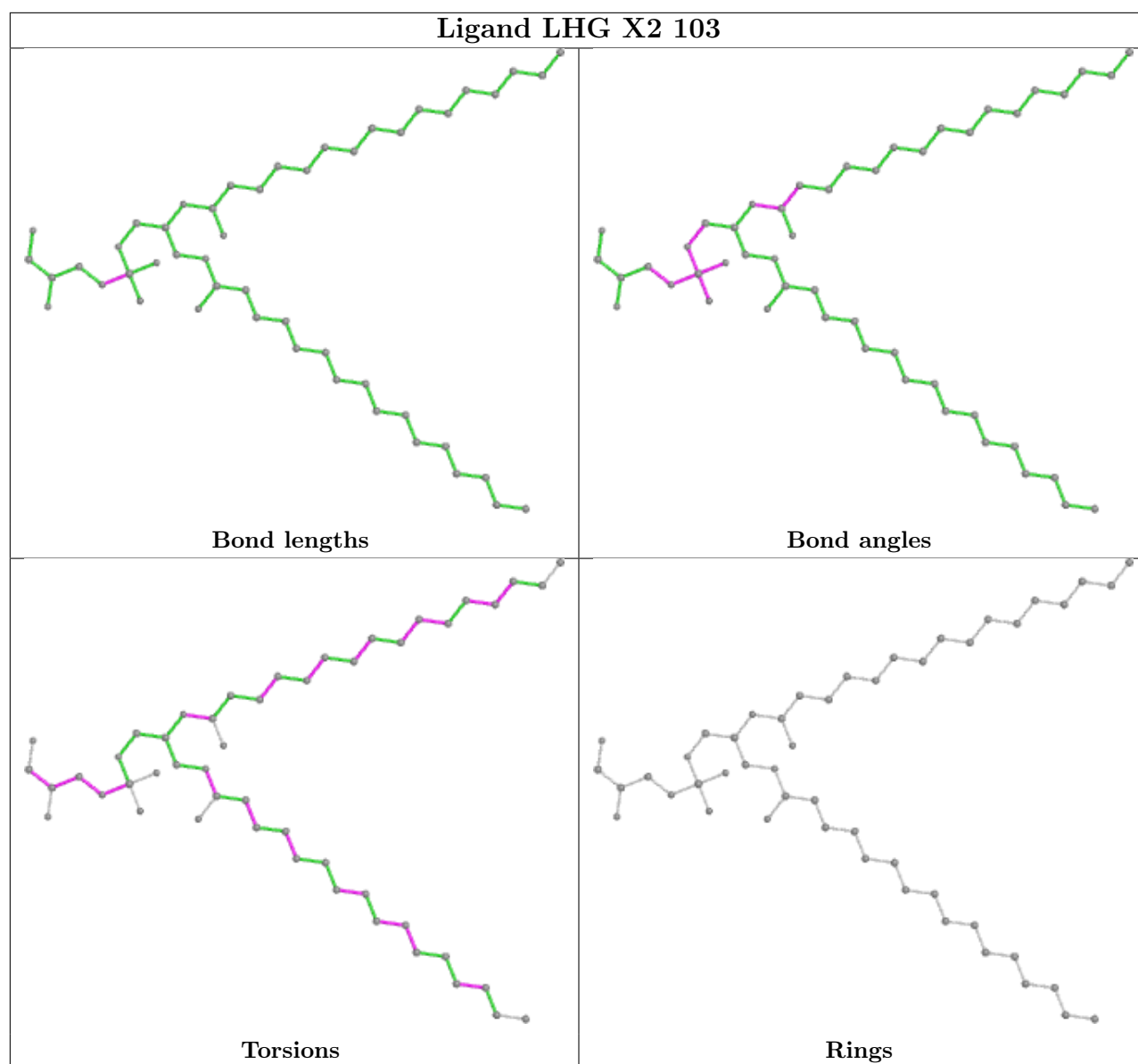




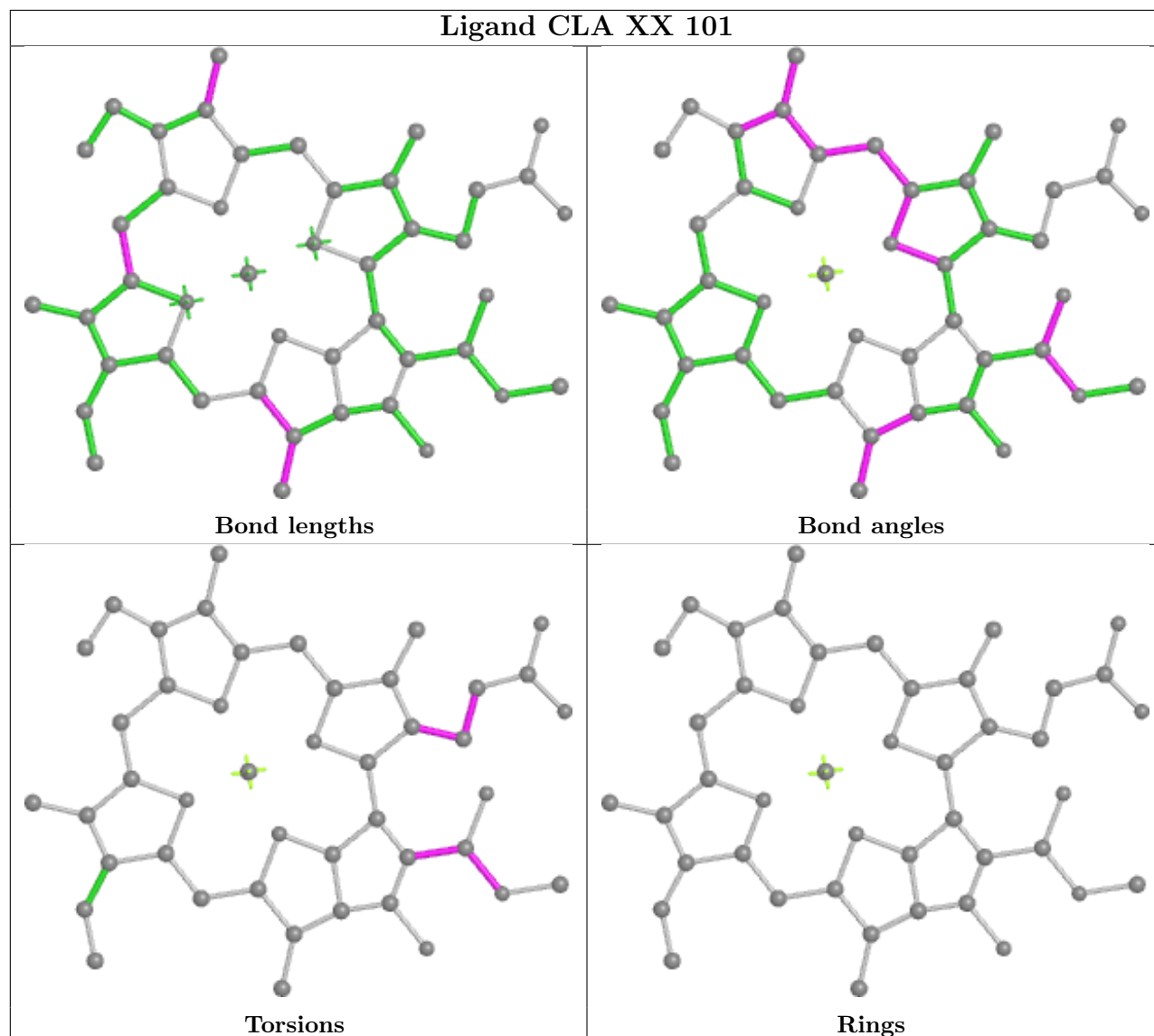
Ligand CLA X2 101

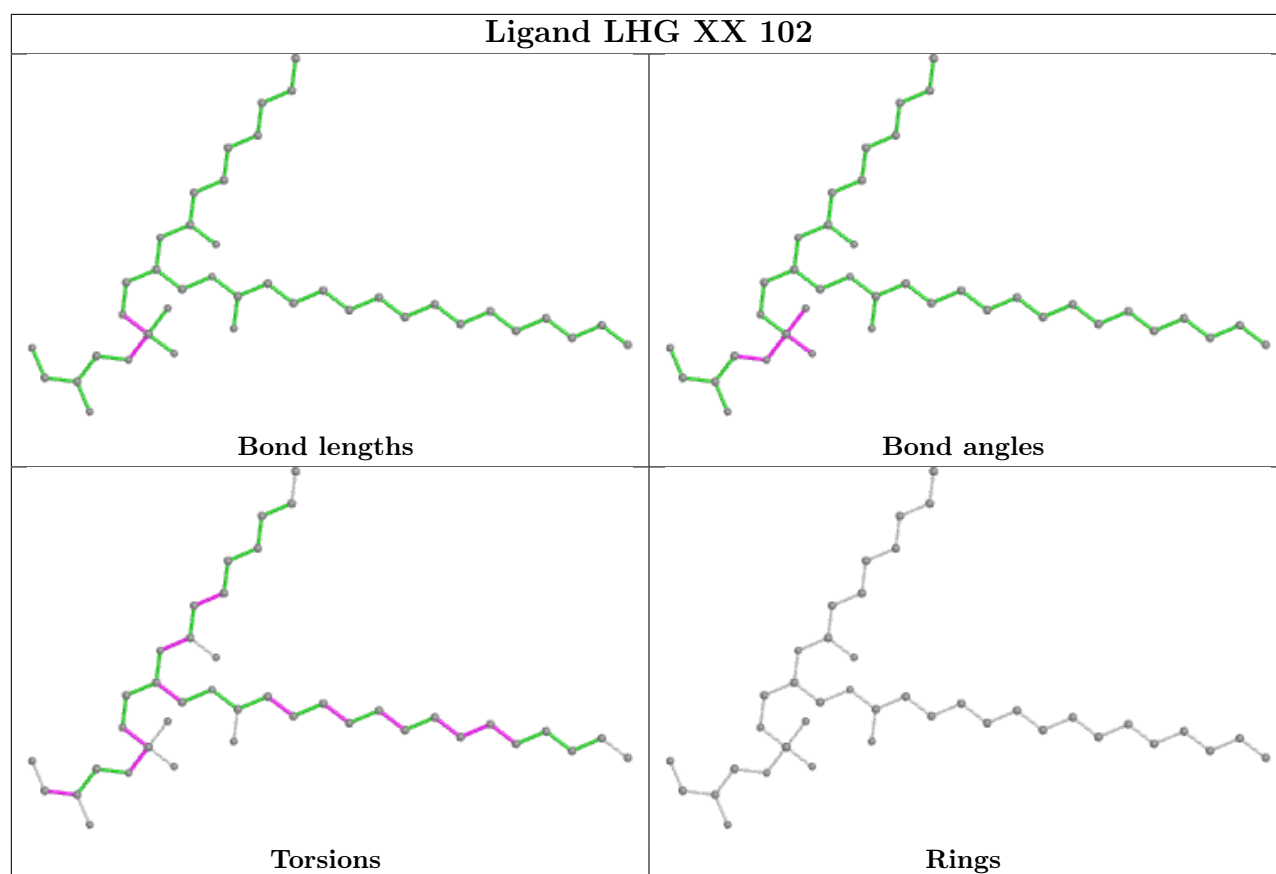






Ligand CLA XX 101





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.